HIGH-END COMPUTING CAPABILITY PORTFOLIO

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NASA Advanced Supercomputing Division

March 10, 2022

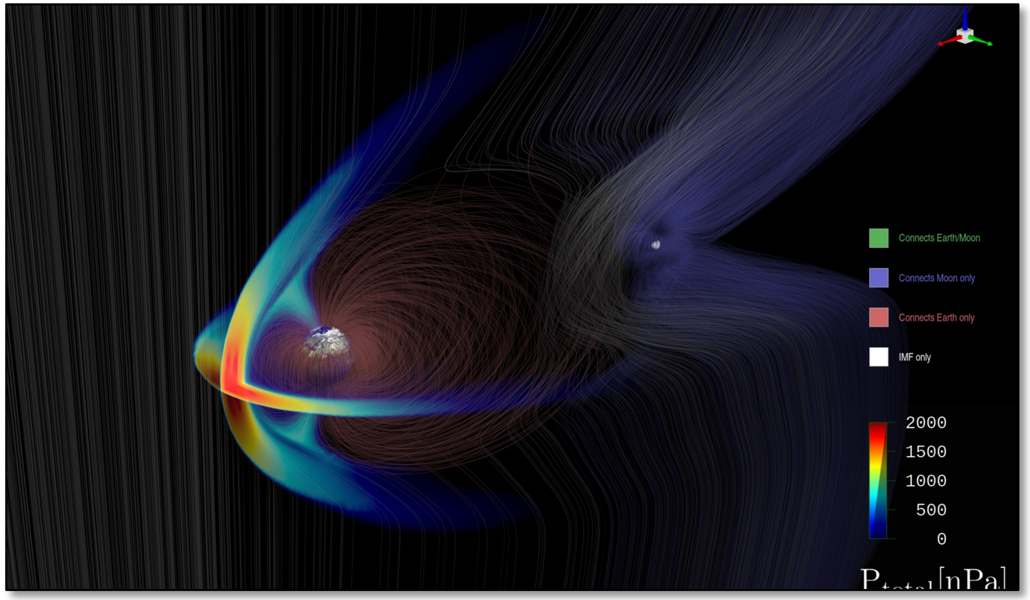
National Aeronautics and Space Administration

HECC Supercomputer Usage Sets New Normalized Record

- In February 2022, the combined usage of HECC supercomputers set a new normalized record of 12,948,515 Standard Billing Units (SBUs).*
- The usage by 420 of NASA's science and engineering groups exceeded the previous record of 12,516,376 SBUs set in January 2022 by 432,139 SBUs.
- The record was achieved in great part by two Science Mission Directorate groups: Earth Science, from coupled Goddard Earth Observing System (GEOS)/Estimating the Circulation and Climate of the Ocean (ECCO) simulations, and Astrophysics, from the Roles Of Stellar Flares And Storms In Exoplanetary Atmospheric Losses And Evolution project.
- Usage of Pleiades, Aitken, Electra, and Endeavour contributed to this record. The new record was enabled by the Aitken Rome nodes, with 128 cores per node.
- The top 10 projects' usage ranged between 234,521 and 861,759 SBUs, and together accounted for over 31% of the total usage.
- The HECC Project continues to evaluate and plan resources to address the future requirements of NASA's users.

** 1 SBU represents the work that can be done in 1 hour on a Pleiades Broadwell 28-core node.*

IMPACT: The increased capacity of HECC systems and working with users to optimize their run capacities provides mission directorates with more resources to accomplish their goals and objectives.



3D representation of the entire magnetized Earth-Moon system during an extreme "Carrington-type" space weather event, where the Moon is behind the Earth. Color contours depict the total fluid pressure in nanoscale, while the cyan lines represent magnetic fields through which oxygen ions can be transported from Earth to the lunar poles. *Chuanfei Dong, Liang Wang, Princeton University*

Request Management System (RMS) Recent Releases

The RMS application development effort made significant progress over the last three months through continuous integration, with four version releases and two “hot fixes”.

- Highlights from the four versions include:
  - Capturing the submit date and history of requests.
  - Adding a new record type “Cancellation” in the history table.
  - Display the funding information for related requests.
  - Developed a Cloud request form prototype.
  - Automatically generate a PDF letter for request summaries to be included in grant requests.
- The new versions also addressed:
  - Functionality improvements.
  - Formatting issues.
  - New fields capturing dates.
  - Communication improvements with RMS users.
- Upcoming versions will improve managing sponsoring organizations, team management (adding and removing team members), and simplified modification compute requests.

IMPACT: Developing in-house software to manage supercomputer resource allocation requests allows NASA’s High End Computing Program more ownership of the data and simplifies the process for reviewing allocations and targets.

National Aeronautics and Space Administration
High-End Computing Program

High-End Computing Request Summary

This request summary will help you meet the requirement of many NASA funding solicitations to upload a PDF version of your completed request to NSPIRES or Grants.gov. Please refer to the specific solicitation for instructions. You can also save this summary for your records.

Date Printed: 2022-02-23

Computational Project Info

HEC Request Number :	
GID:	
Title:	
Principal Investigator:	
Organization:	
Justification:	
Duration:	

Funding Source Info

Sponsoring NASA Organization:	
Funding Source:	
Solicitation Number:	
NASA WBS/Contract/Grant #:	
Funding Manager:	

Desired Resource Info

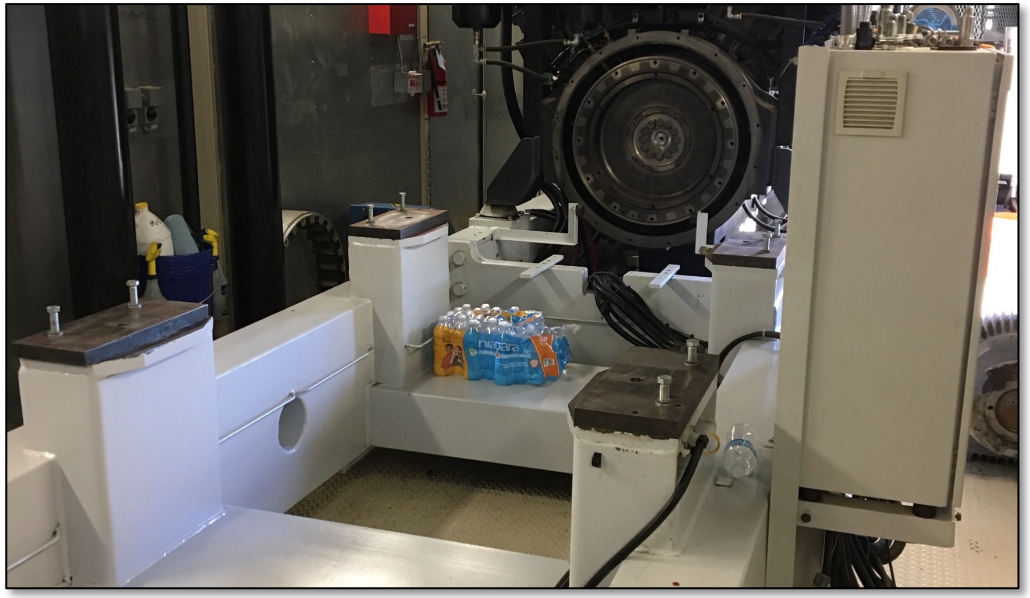
Fiscal Year	Location	Requested SBUs	Allocated SBUs	Date Allocated
2021	HECC	43,869	43,869	2022-04-09
2022	HECC	350,000	350,000	2021-09-07
2022	HECC	400,000	TBD	TBD

Redacted example of the new letter for request summary sent to requestors automatically from the Resource Management System. These letters are required for grants. *NASA*

Two RUPS Units Receive Major Maintenance Services

- Maintenance upgrades were completed on two of the three Rotary Uninterruptible Power Supply (RUPS) supporting Building N258.
- RUPS #2 and #3 underwent their scheduled five-year refurbishments, which included detailed maintenance on the RUPS major subsystems: generator, diesel engine, and induction coupling (IC).
  - In addition, RUPS #2 received a new IC in January 2022 to replace the existing IC that had a bearing failure.
  - RUPS #1 was excluded from the major maintenance effort, as it received its five-year refurbishment in 2018 and a new IC in 2020; but during an inspection, a hole was discovered in the diesel engine's muffler. The repair is scheduled for next month.
- The three RUPS units run in parallel to provide uninterruptible, conditioned power to Pleiades, data storage systems, and the N258 data center cooling system.
- Currently, the RUPS is 2+0 (also called the "N configuration") to provide UPS protection for HECC filesystems and cooling, with full RUPS protection of all N258 HECC resources to be in place after the RUPS #1 repair.

IMPACT: Protecting HECC resources at NASA's largest supercomputing facility provides reduced risk of failure due to power outage events and increases resource availability for NASA users.



The RUPS 3000-horsepower diesel engine with the induction coupling removed from the support frame. *Chris Tanner, NASA/Ames*

Chandra Simulations Used to Create ‘Galactic Center’ Virtual Reality App*

- Using models simulating the black hole and stars at the center of the Milky Way, researchers at the University of Delaware and Catholic University of America ran simulations on Pleiades to explain observations from NASA’s Chandra X-ray Observatory and created a virtual reality (VR) app that lets users fly through the center of the Milky Way.
  - The simulations are validated by computing their X-ray emission (both X-ray spectra and X-ray images) to compare directly with the Chandra observations.
  - The “Galactic Center VR” app allows users to explore the simulations using VR, which provides a unique method of exploring complex multi-dimensional datasets due to the ability to immerse the user within the dataset.
- The simulations are in close agreement with Chandra observations of Earth’s nearest supermassive black hole (Sgr A*) and its surrounding region. A reservoir of hot gas is well explained by the winds from 25 Wolf-Rayet stars orbiting the black hole. This provides confidence that other results from the simulations that are not directly observable, such as the flow of wind material towards the black hole, are accurate.
- The team was recently awarded funding from the Chandra program to add ~ 65 more stars and their winds to the simulations and to upgrade the X-ray calculations to include the Doppler shift of the hot gas. Results should provide the most complete picture to date of how the massive stars orbiting Sgr A* feed the black hole via their stellar winds.

IMPACT: HECC resources are essential to the workflow of this Chandra-funded project: simulations tests, production runs, analysis tasks, construction of 360-degree videos, and reformatting of output files for VR.

This screenshot from inside the virtual reality (VR) headset shows the supermassive black hole at the center of the Milky Way Galaxy, including the stars with their orbit lines drawn and the colliding winds (red and yellow) with their X-ray emission (blue and cyan) within a few light years of the black hole. *Christopher Russell, University of Delaware & Catholic University of America*

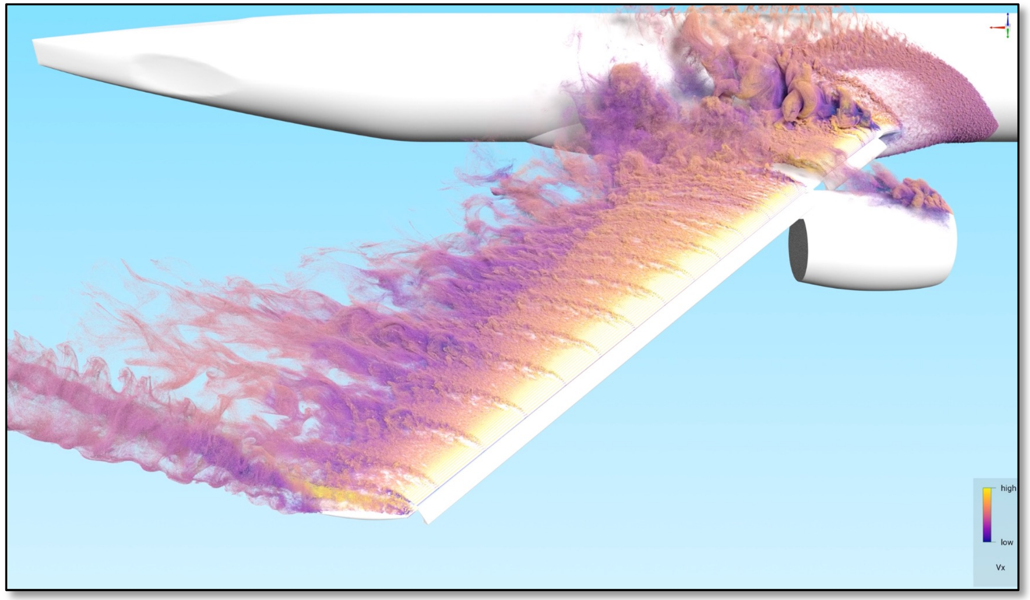
** HECC provided supercomputing resources and services in support of this work.*

Simulations for Aircraft Certification by Analysis*

- High-lift vehicle simulations pose a major challenge for current computational fluid dynamics (CFD) algorithms due to the highly chaotic nature of the separated flows in these configurations. Separated flows have length and time scales that are strongly influenced by the vehicle geometry, and legacy models using Reynolds-Averaged Navier-Stokes (RANS) solutions—which rely on calibration—often fail in these flow types.
- In order to address NASA's current CFD software shortcomings, the Launch Ascent and Vehicle Aerodynamics (LAVA) group at NASA's Ames Research Center has been researching the development and assessment of cutting-edge numerical technologies, eventually enabling new aircraft Certification by Analysis methods.
- The group used the High-Lift Common Research Model as a benchmark to develop scale-resolving algorithms within the LAVA framework. They were able to show that Wall-Modeled Large-Eddy Simulations (WMLES) methods with LAVA do not suffer from the same drawbacks as RANS-based solutions.
- Since scale-resolving algorithms like WMLES require more computational resources than RANS methods, the LAVA team aimed to ensure that the high-lift configuration was able to perform efficiently on the Pleiades, Electra, and Aitken supercomputers at the NASA Advanced Supercomputing (NAS) facility, including developing new load balancing features to allow simulations with more than 275 million grid points to run in less than eight hours.

** HECC provided supercomputing resources and services in support of this work.*

IMPACT: The advancement of CFD methods toward Certification by Analysis will relieve some of the high financial burden of wind tunnel and flight testing for new aircraft designs.



Particle traces illustrate the flow topology on the suction side of a wing at an angle of attack of 21.5 degrees. The particle trajectories on the outboard part of the wing show the role of slat brackets/attachments at inducing separation, and strong corner flow separation is observed near the wing-body juncture. Particles are colored by velocity.
Timothy Sandstrom, NASA/Ames

Papers

- “**TOI-1759 b: A Transiting Sub-Neptune Around a Low Mass Star Characterized with SPIRou and TESS**,” E. Martioli, et al., arXiv:2202.01259 [astro-ph.EP], February 2, 2022. *
  https://arxiv.org/abs/2202.01259
- “**Automated Processing of X-Ray Computed Tomography Images via Panoptic Segmentation for Modeling Woven Composite Textiles**,” A. Allred, L. Abbot, A. Doostan, K. Maute, arXiv:2202.01265 [cs.CV], February 2, 2022. *
  https://arxiv.org/abs/2202.01265
- “**Improving the Alfvén Wave Solar Atmosphere Model Based on Parker Solar Probe Data**,” B. van der Holst, et al., The Astrophysical Journal, vol. 925, no. 2, February 2, 2022. *
  https://iopscience.iop.org/article/10.3847/1538-4357/ac3d34/meta
- “**Tidal Simulation Revisited**,” W. Huang, et al., Ocean Dynamics (Springer), February 5, 2022. *
  https://link.springer.com/article/10.1007/s10236-022-01498-9
- “**Longitudinally Modulated Dynamo Action in Simulated M-Dwarf Stars**,” C. Bice, J. Toomre, arXiv:2202.02869 [astro-ph.SR], February 6, 2022. *
  https://arxiv.org/abs/2202.02869
- “**A Collisional Test-Particle Model of Electrons at a Comet**,” P. Stephenson, et al., Monthly Notices of the Royal Astronomical Society, vol. 511, issue 3, published online February 7, 2022. *
  https://academic.oup.com/mnras/article/511/3/4090/6523370?login=true

** HECC provided supercomputing resources and services in support of this work*

Papers (cont.)

- "**Charge State Calculation for Global Solar Wind Modeling**," J. Szente, et al., The Astrophysical Journal, vol. 926, no. 1, February 9, 2022. *
  https://iopscience.iop.org/article/10.3847/1538-4357/ac3918
- "**97 Eclipsing Quadruple Star Candidates Discovered in TESS Full Frame Images**," V. Kostov, et al., arXiv:2202.05790 [astro-ph.SR], February 11, 2022. *
  https://arxiv.org/abs/2202.05790
- "**Indian Monsoon Teleconnections and the Impact of Correcting Tropical Diabatic Heating**," E. Swenson, D. Straus, D. Das, Journal of Atmospheric Sciences, published online February 14, 2022. *
  https://journals.ametsoc.org/view/journals/atsc/aop/JAS-D-21-0231.1/JAS-D-21-0231.1.xml
- "**NEID Rossiter-McLaughlin Measurement of TOI-1268b: A Young Warm Saturn Aligned with its Cool Host Star**," J. Dong, et al., The Astrophysical Journal Letters, vol. 926, no. 2, February 16, 2022. *
  https://iopscience.iop.org/article/10.3847/2041-8213/ac4da0/meta
- "**A Transiting, Temperate Mini-Neptune Orbiting the M-Dwarf TOI-1759 Unveiled by TESS**," N. Espinoza, et al., The Astronomical Journal, vol. 163, no. 3, February 16, 2022. *
  https://iopscience.iop.org/article/10.3847/1538-3881/ac4af0/meta
- "**TOI-2119: A Transiting Brown Dwarf Orbiting an Active M-Dwarf from NASA's TESS Mission**," T. Carmichael, et al., arXiv:2202.08842 [astro-ph.SR], February 17, 2022. *
  https://arxiv.org/abs/2202.08842

** HECC provided supercomputing resources and services in support of this work*

Papers (cont.)

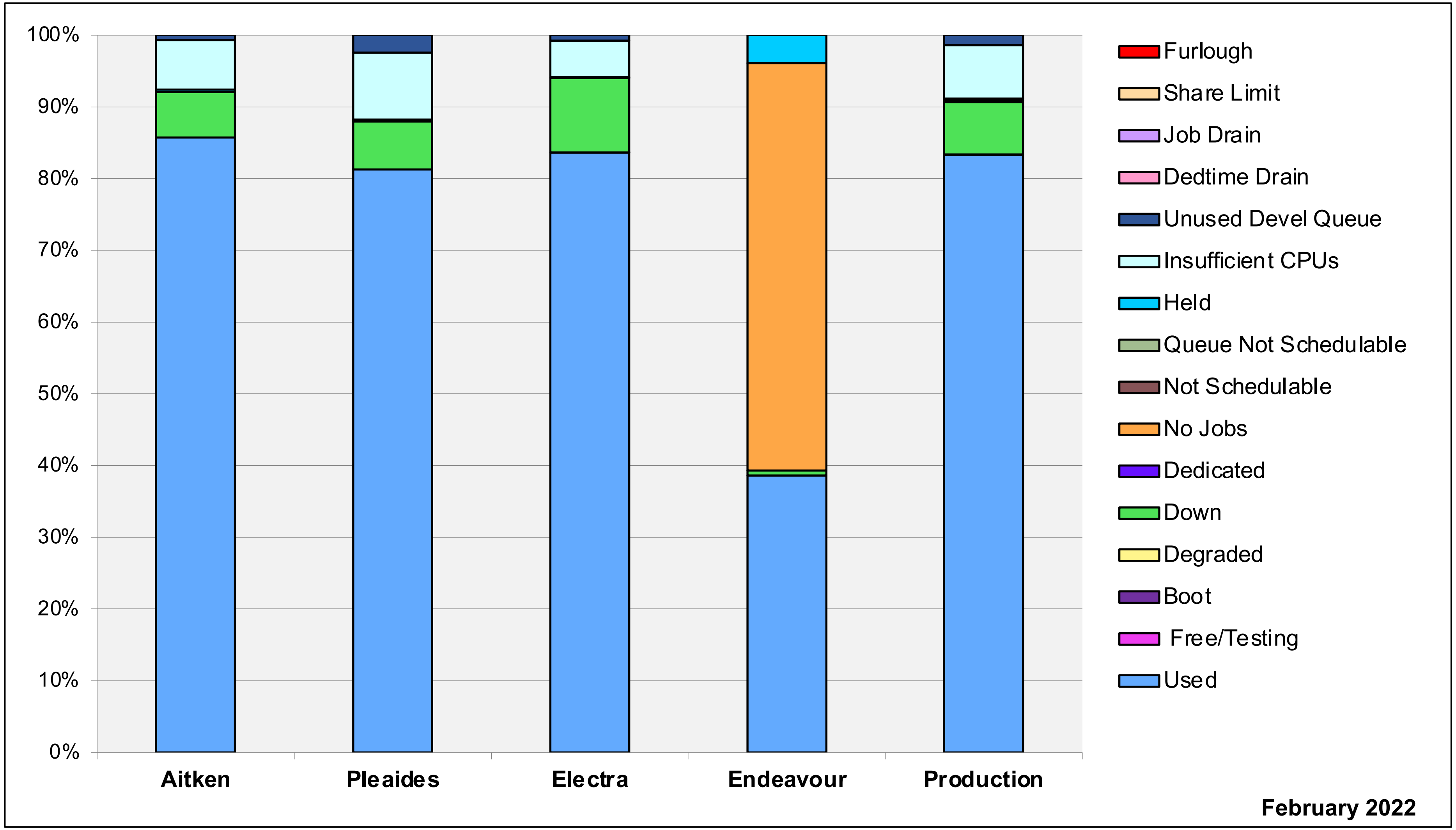
- "**Mixing of Condensable Constituents with H-He During the Formation& Evolution of Jupiter**," D. Stevenson, et al., arXiv:2202.09476 [astro-ph.EP], February 18, 2022. *
  https://arxiv.org/abs/2202.09476
- "**TESS Discovery of a Sub-Neptune Orbiting a Mid-M-Dwarf TOI-2136**," T. Gan, et al., arXiv:2202.10024 [astro-ph.EP], February 21, 2022. *
  https://arxiv.org/abs/2202.10024
- "**Grand Canonical Monte Carlo Simulations of the Hydrogen Storage Capacities of Slit-Shaped Pores, Nanotubes, and Torusenes**," D. Caviedes, I. Cabria, International Journal of Hydrogen Energy, published online February 25, 2022. *
  https://www.sciencedirect.com/science/article/pii/S0360319922004736
- "**The Reliability of the Small-Core Lanthanide Effective Core Potentials**," C. Bauschlicher Jr., Theoretical Chemistry Accounts, vol. 141, February 26, 2022. *
  https://link.springer.com/article/10.1007/s00214-022-02867-9
- "**Direct Numerical Simulation of Acoustic Disturbances in a Hypersonic Two-Dimensional Nozzle Configuration**," N. Hildebrand, et al., AIAA Journal, published online February 28, 2022. *
  https://arc.aiaa.org/doi/abs/10.2514/1.J061053?journalCode=aiaaj
- "**Potential Link Between Ice Nucleation and Climate Model Spread in Arctic Amplification**," I. Tan, D. Barahona, Q. Coopman, Geophysical Research Letters, vol. 49, issue 4, February 28, 2022. *
  https://agupubs.onlinelibrary.wiley.com/doi/full/10.1029/2021GL097373

** HECC provided supercomputing resources and services in support of this work*

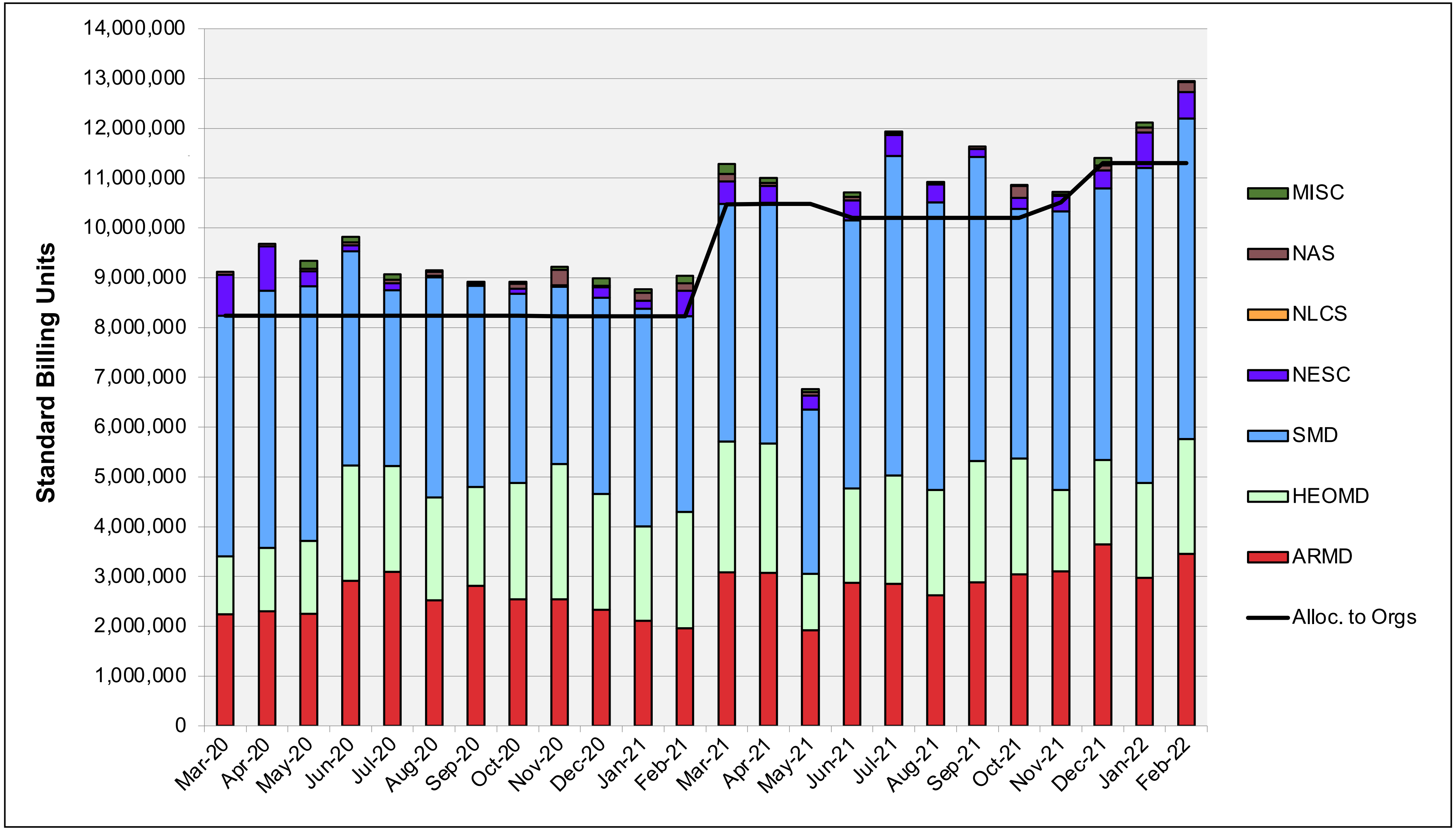
News and Events: Social Media

- **Coverage of NAS Stories**
  - Artemis Booster Separation Image Feature (Ames):
    - NASA Ames: Twitter 115 retweets, 13 quote tweets, 675 likes; Facebook, 104 likes, 4 comments, 23 shares.
    - NASA Supercomputing: Twitter 5 retweets, 36 likes; Facebook 915 users reached, 34 engagements, 13 likes, 1 share.

HECC Utilization



HECC Utilization Normalized to 30-Day Month



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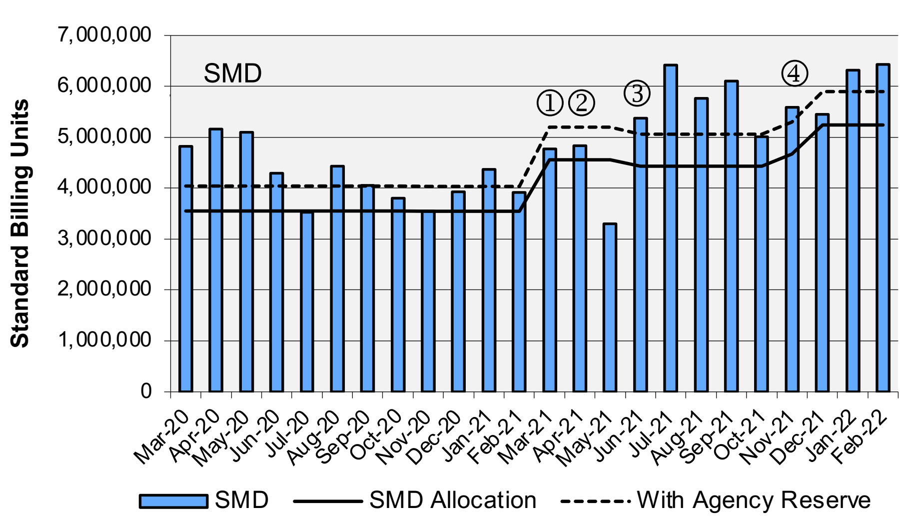
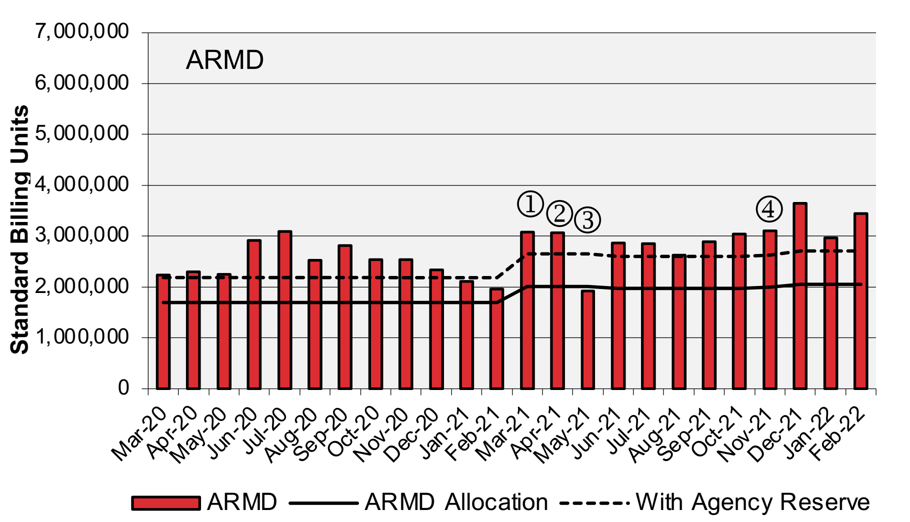
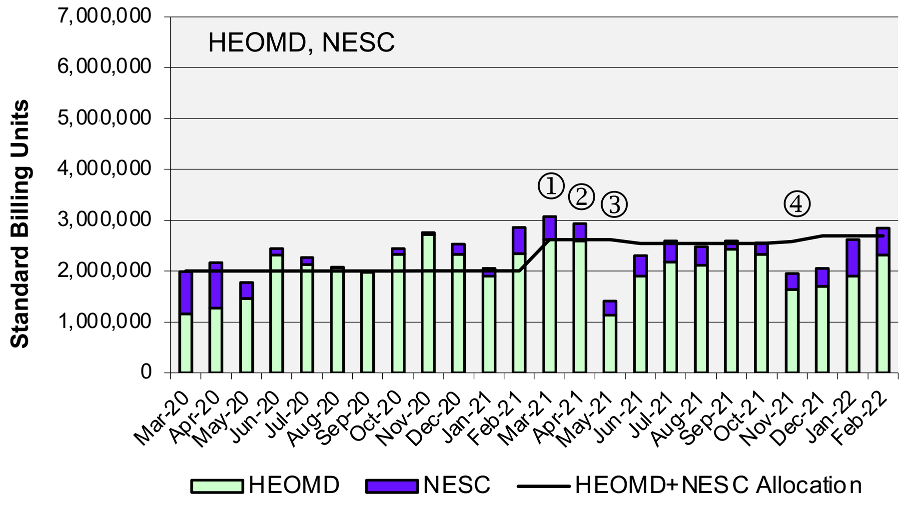






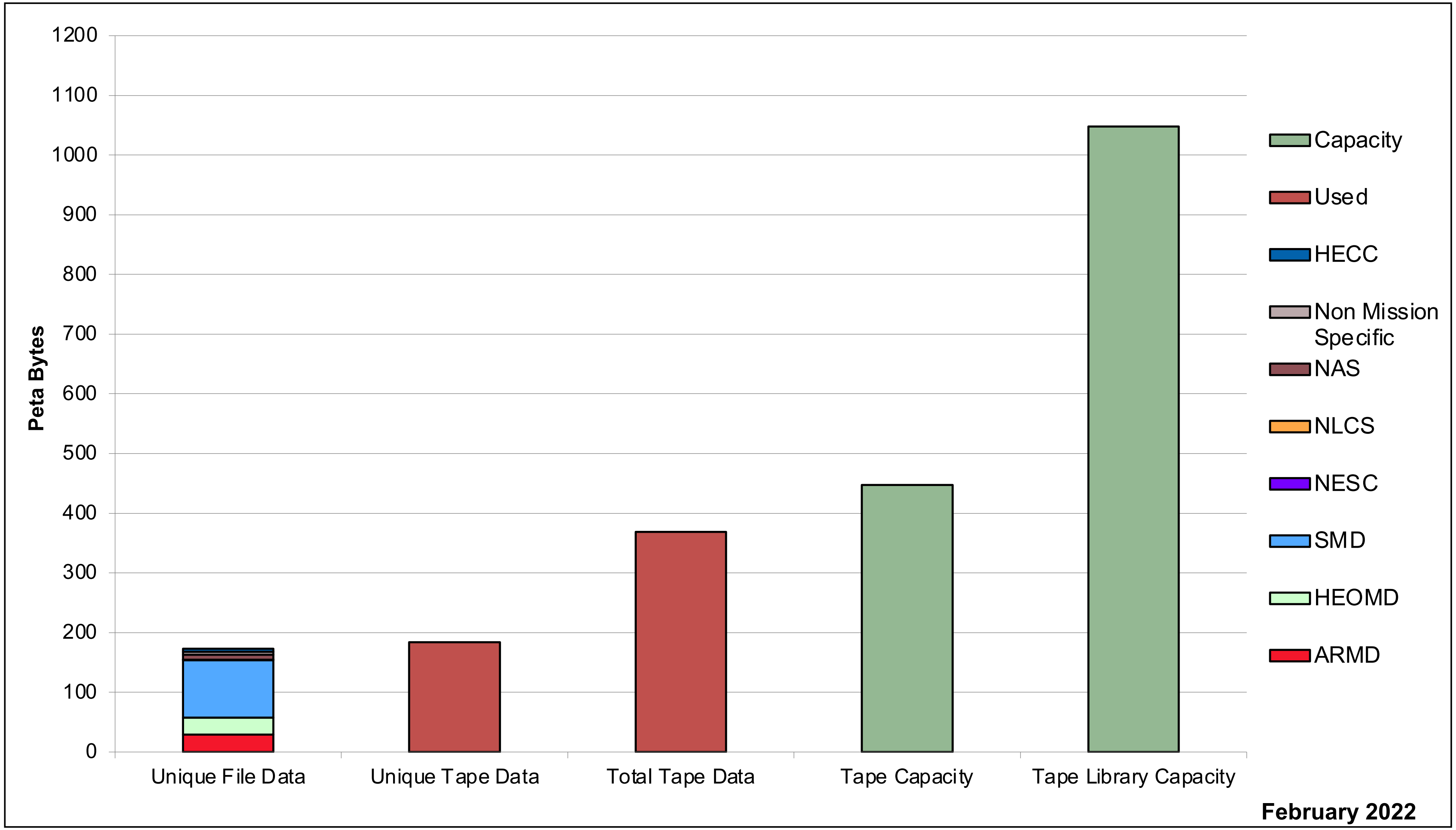
① 8 Rome Apollo racks introduced into Aitken

② Endeavour replaced with new hardware

③ Merope retired

④ 4 Rome Apollo Racks added to Aitken

Tape Archive Status



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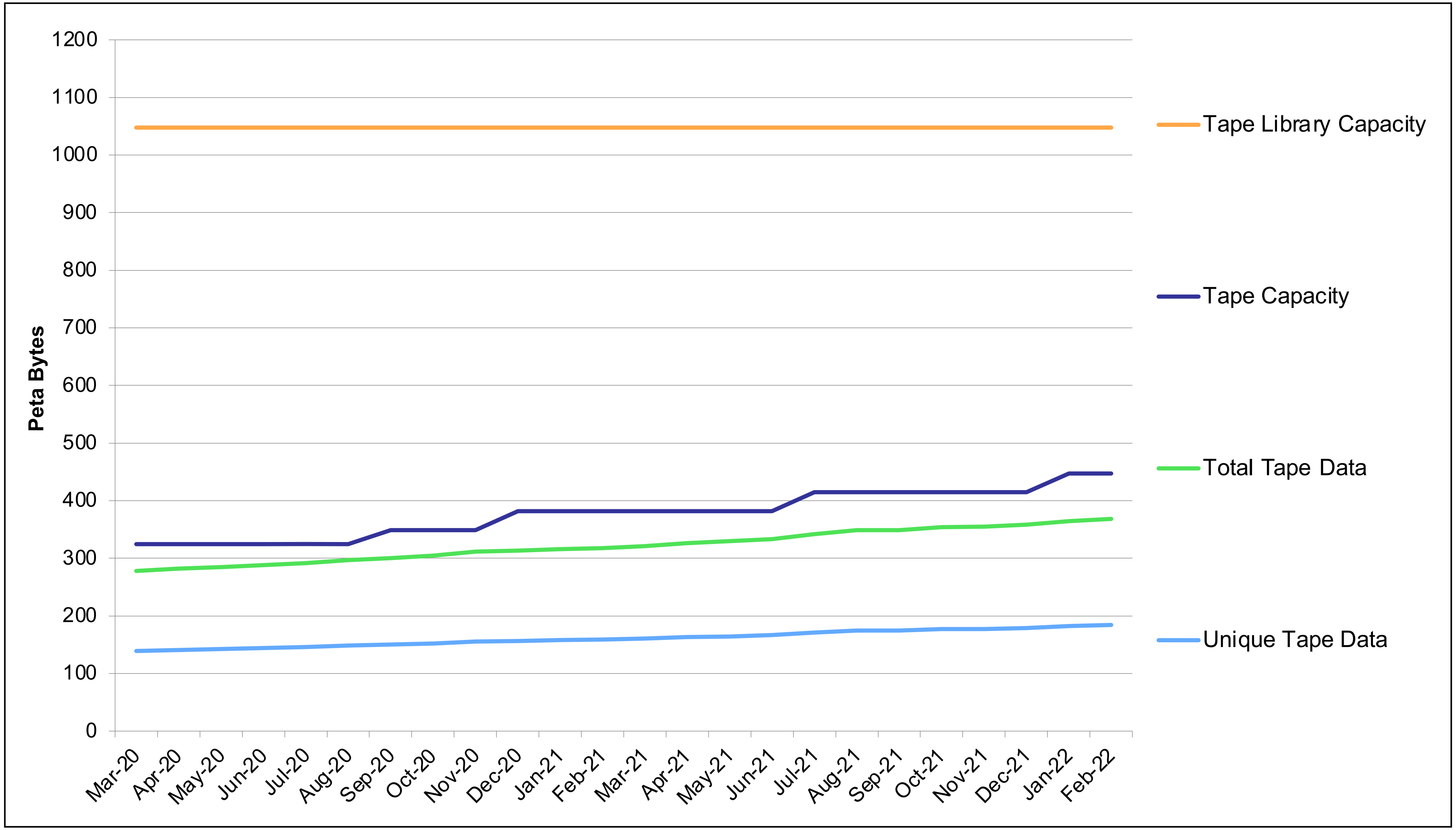
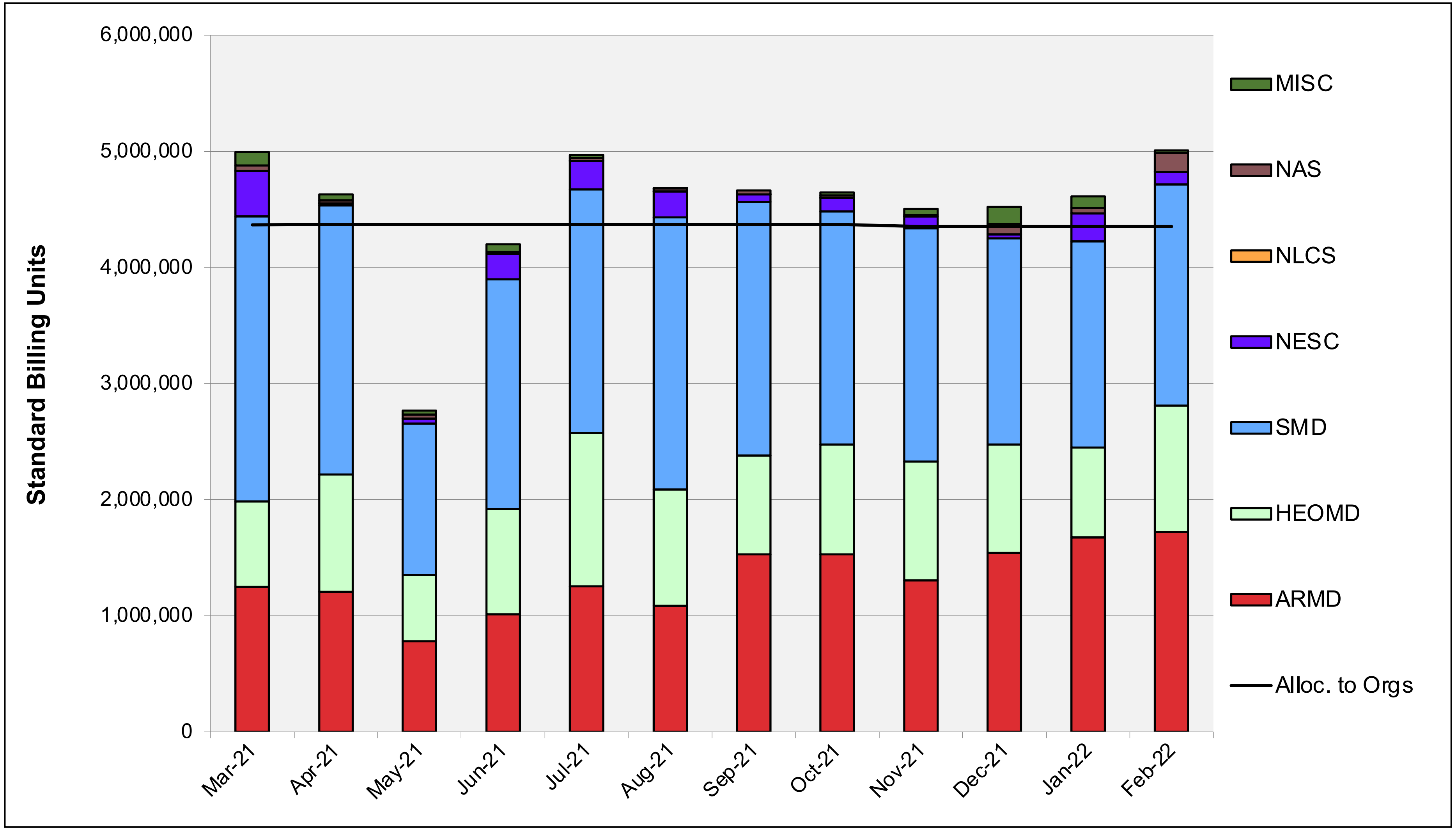
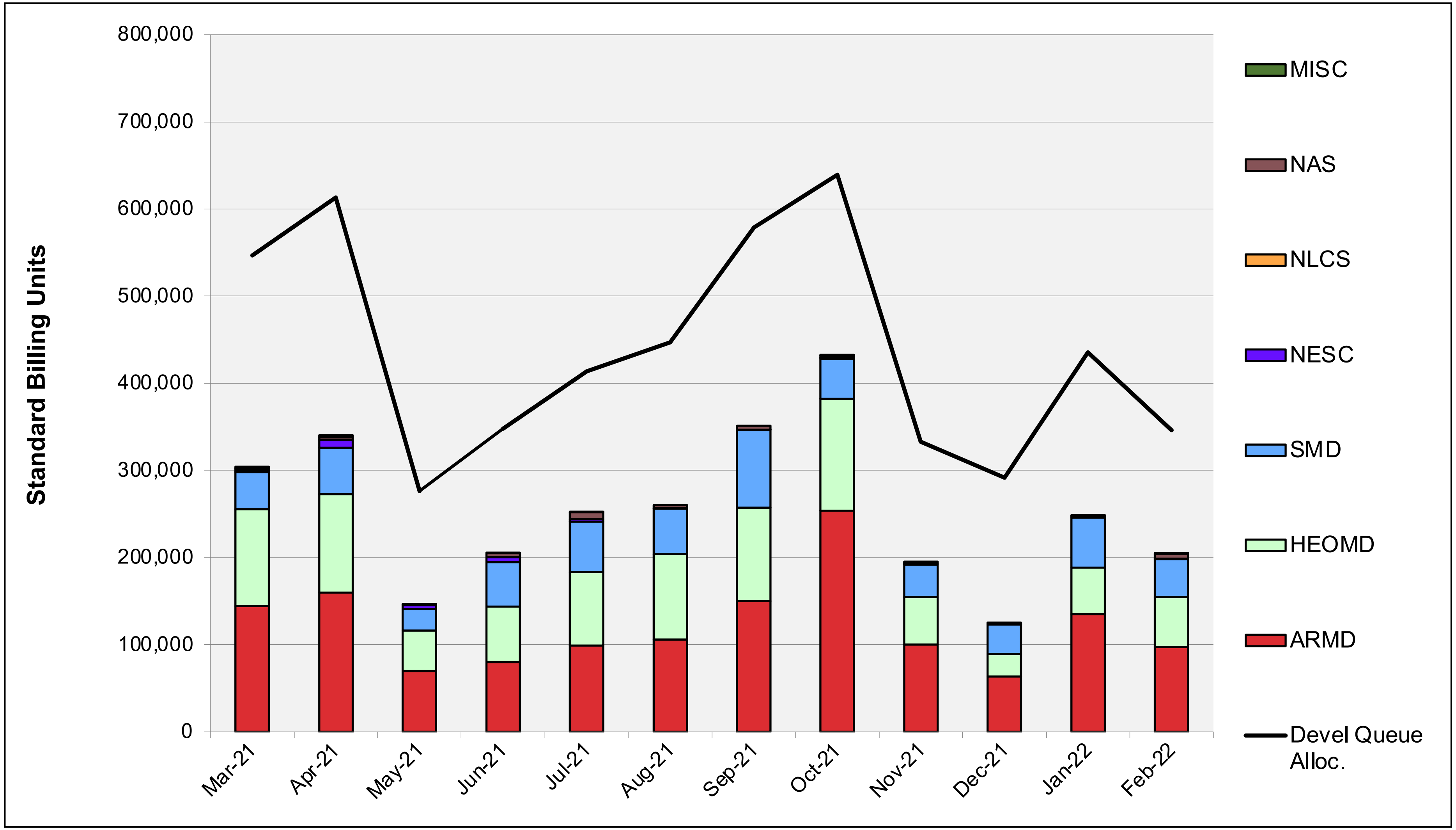


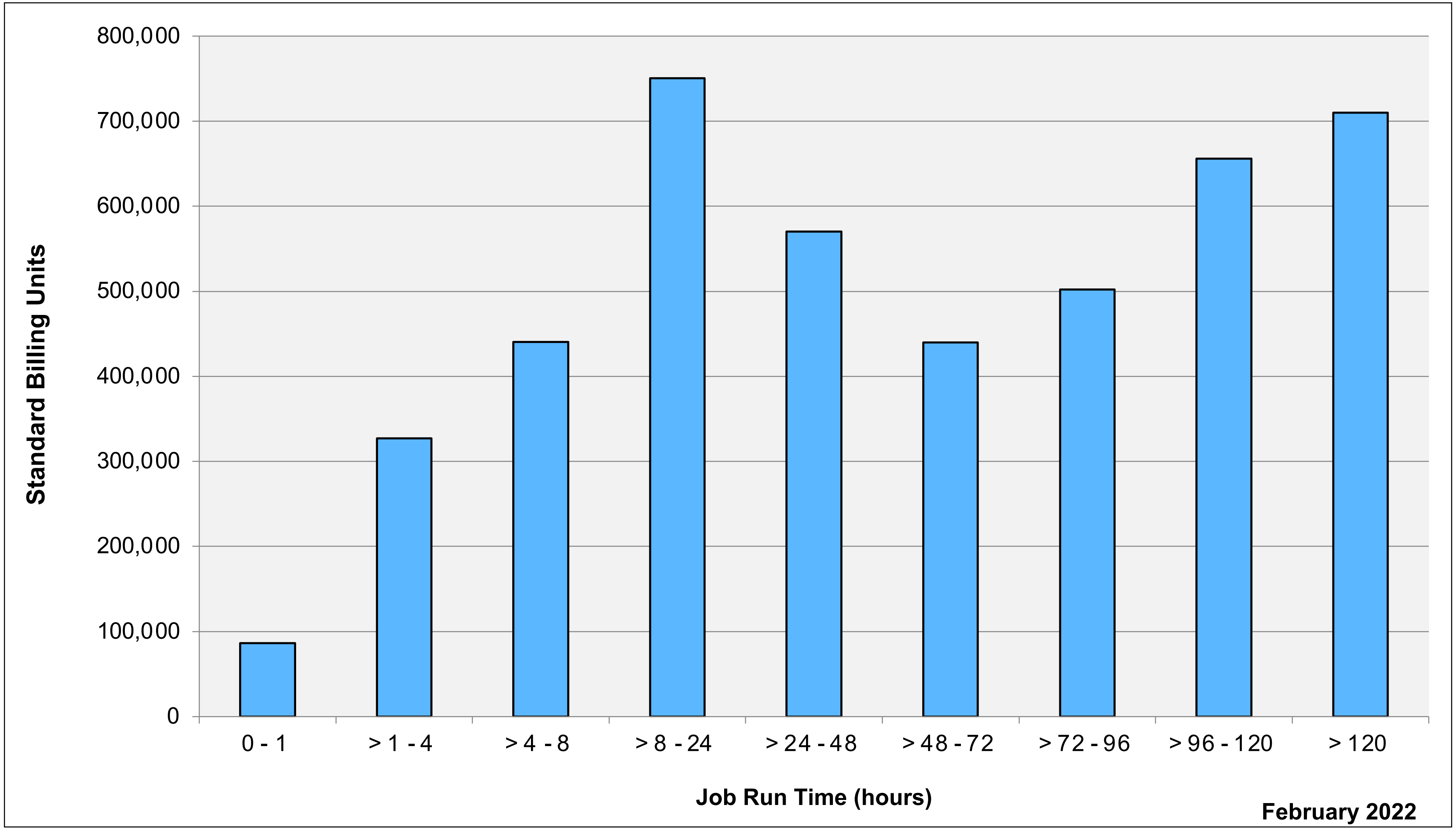
Pleiades: SBUs Reported, Normalized to 30-Day Month



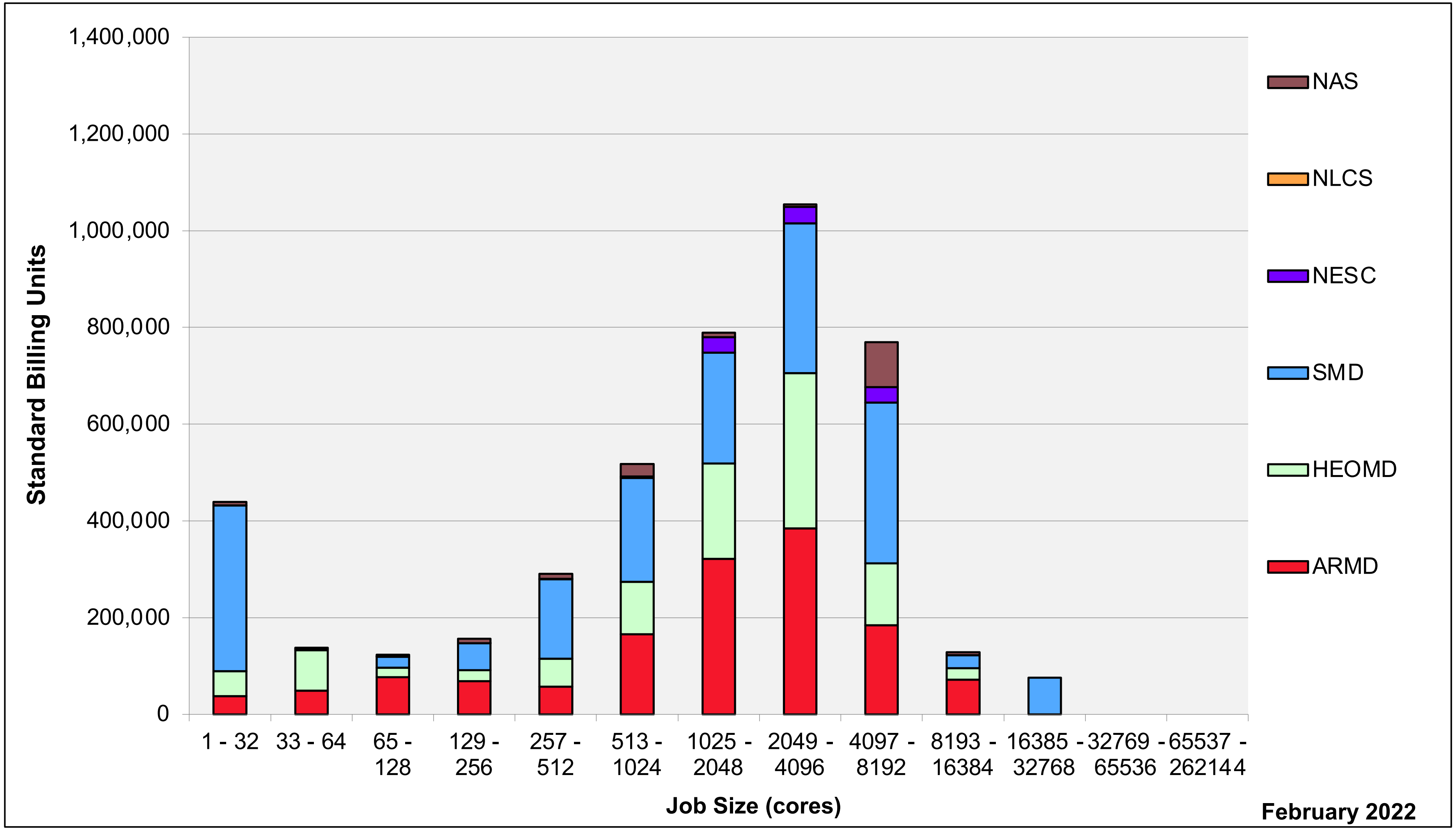
Pleiades: Devel Queue Utilization



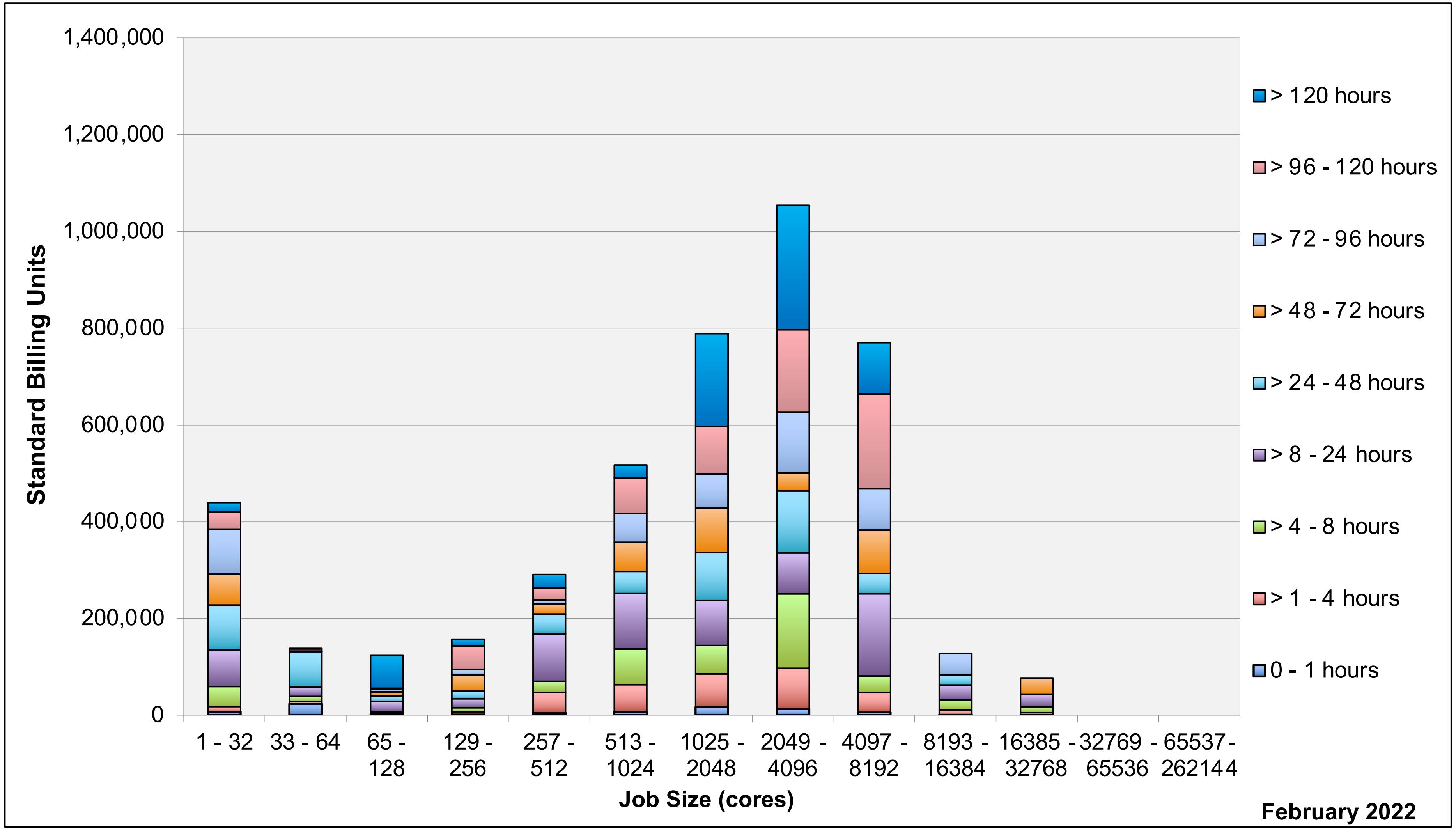
Pleiades: Monthly Utilization by Job Length



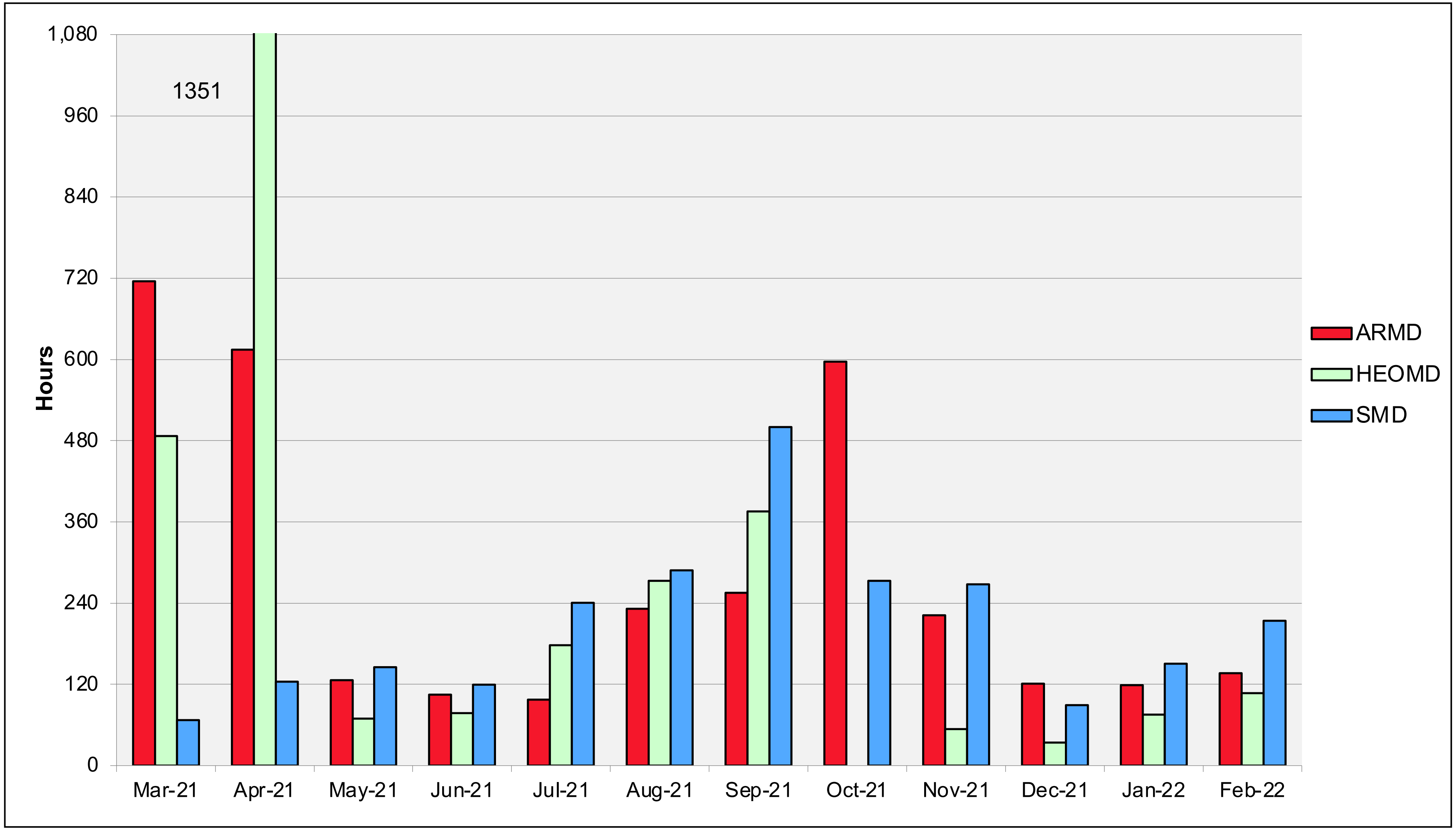
Pleiades: Monthly Utilization by Job Size



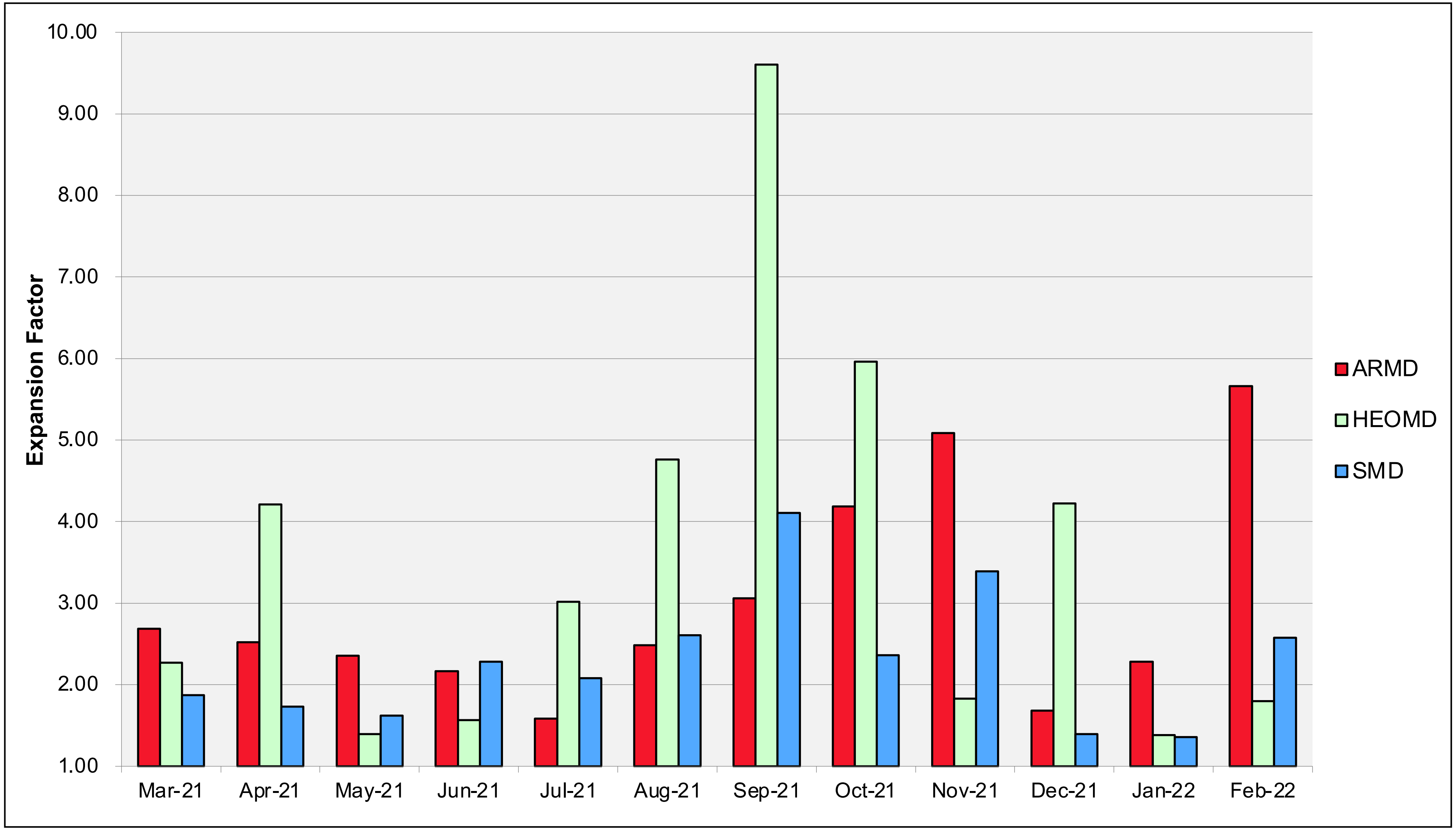
Pleiades: Monthly Utilization by Size and Length



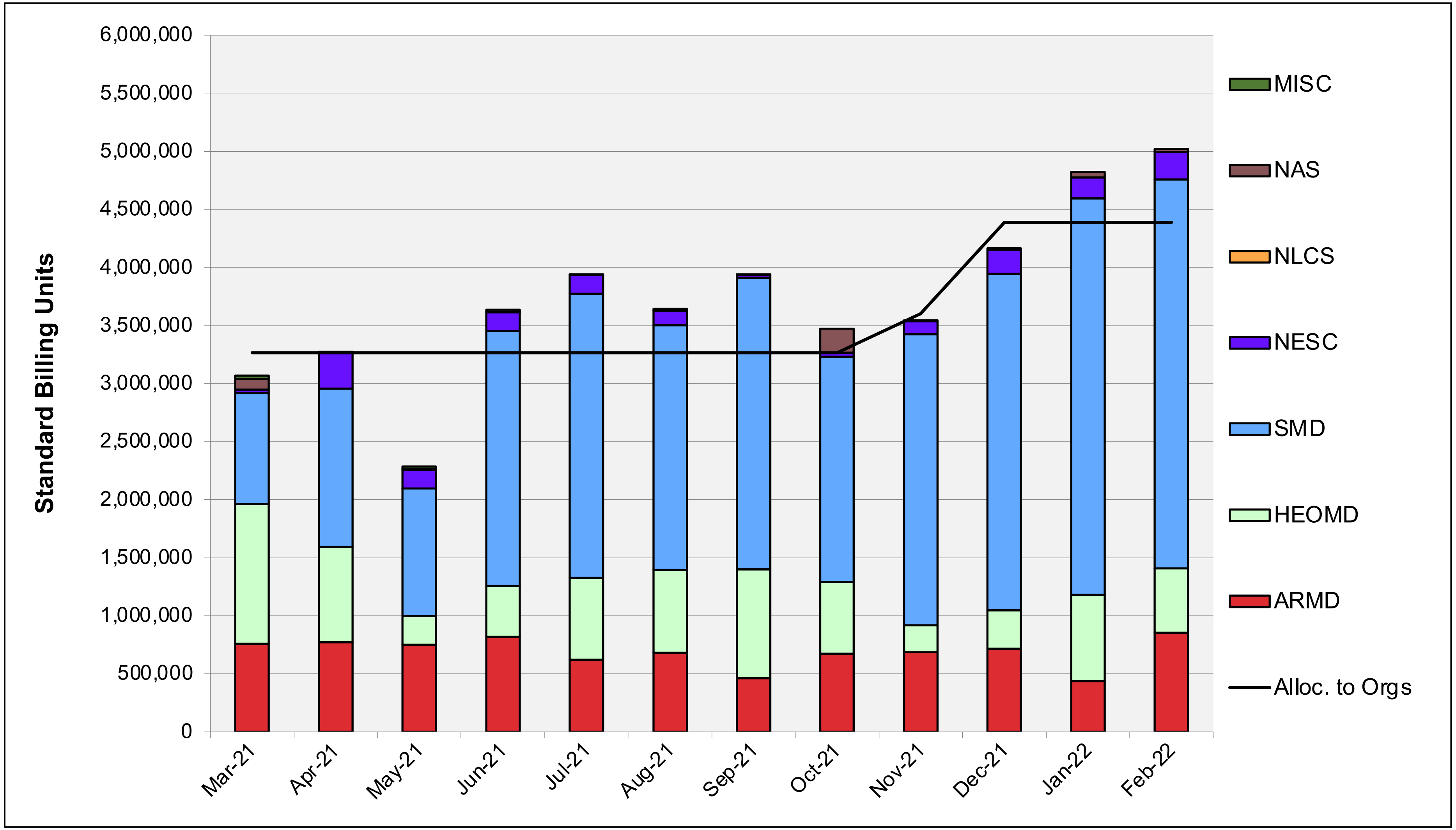
Pleiades: Average Time to Clear All Jobs



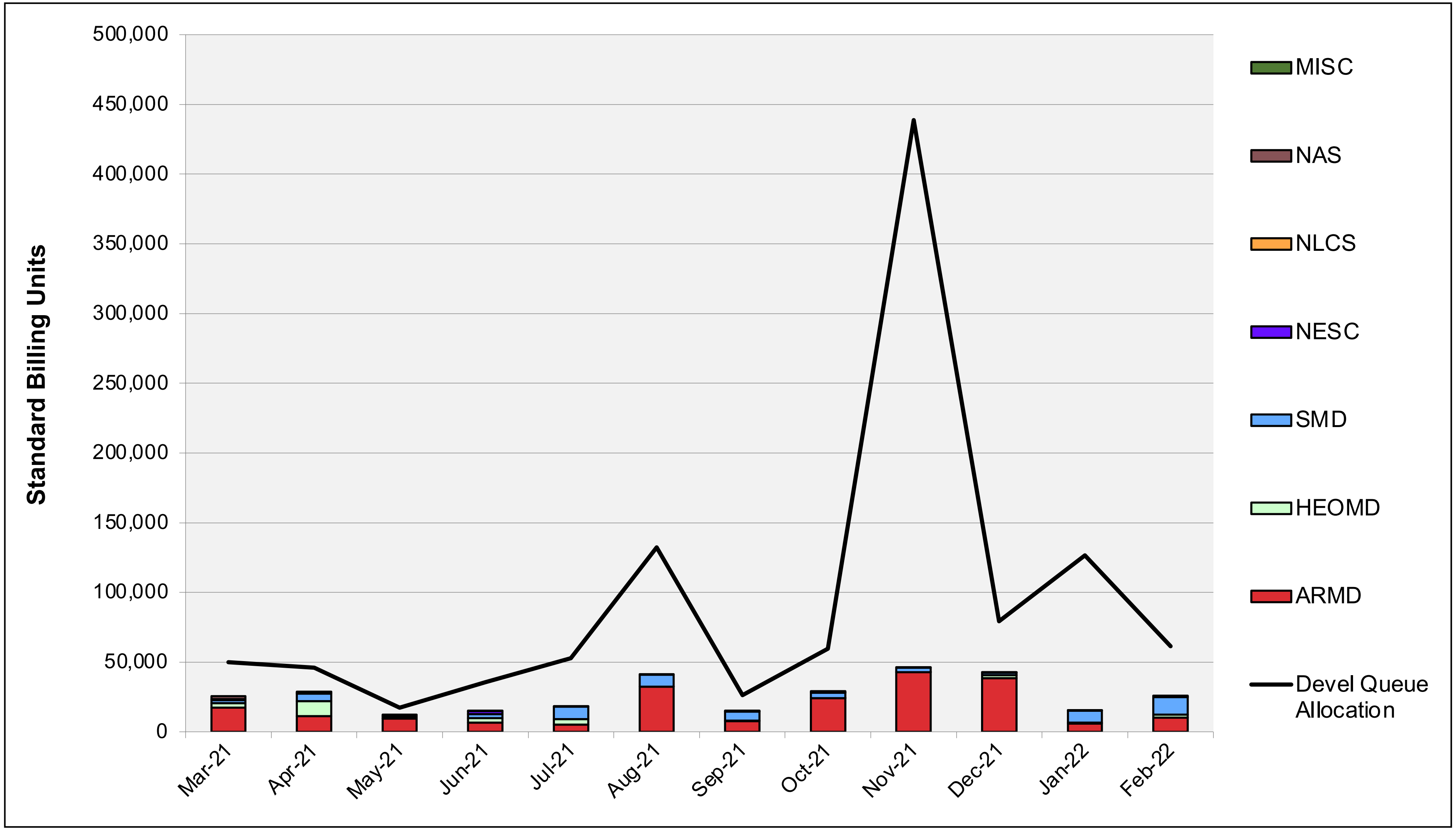
Pleiades: Average Expansion Factor



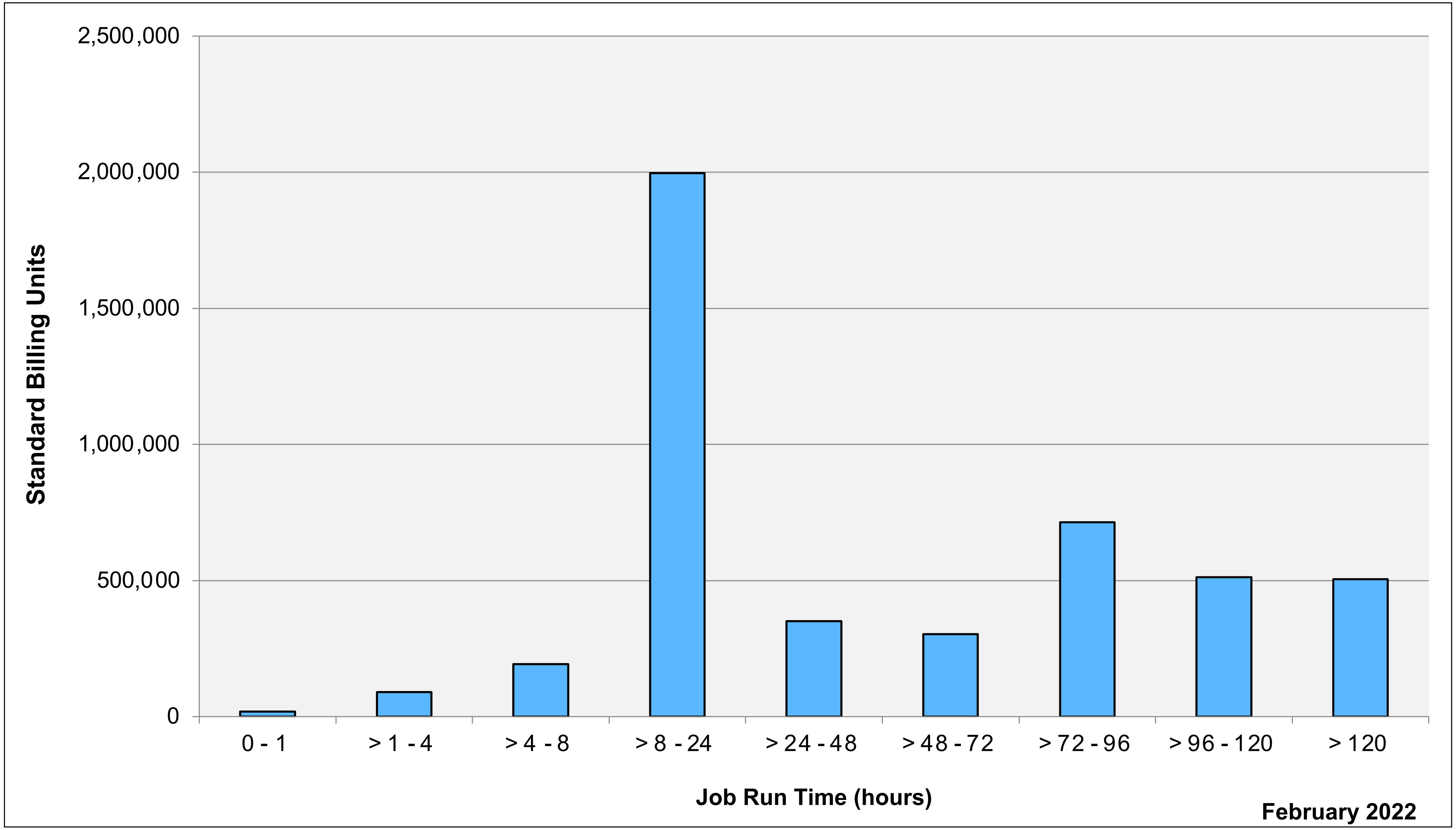
Aitken: SBUs Reported, Normalized to 30-Day Month



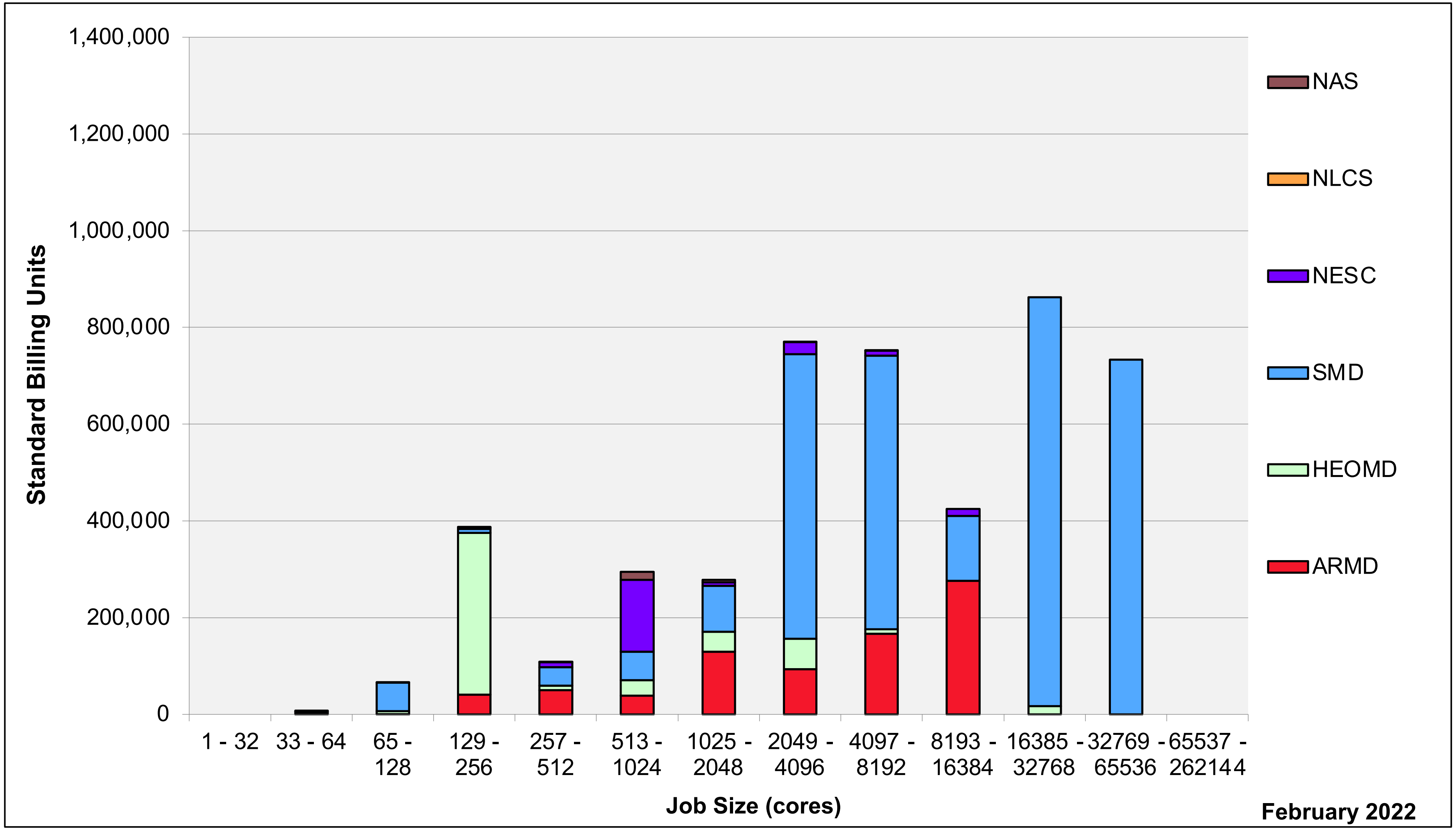
Aitken: Devel Queue Utilization



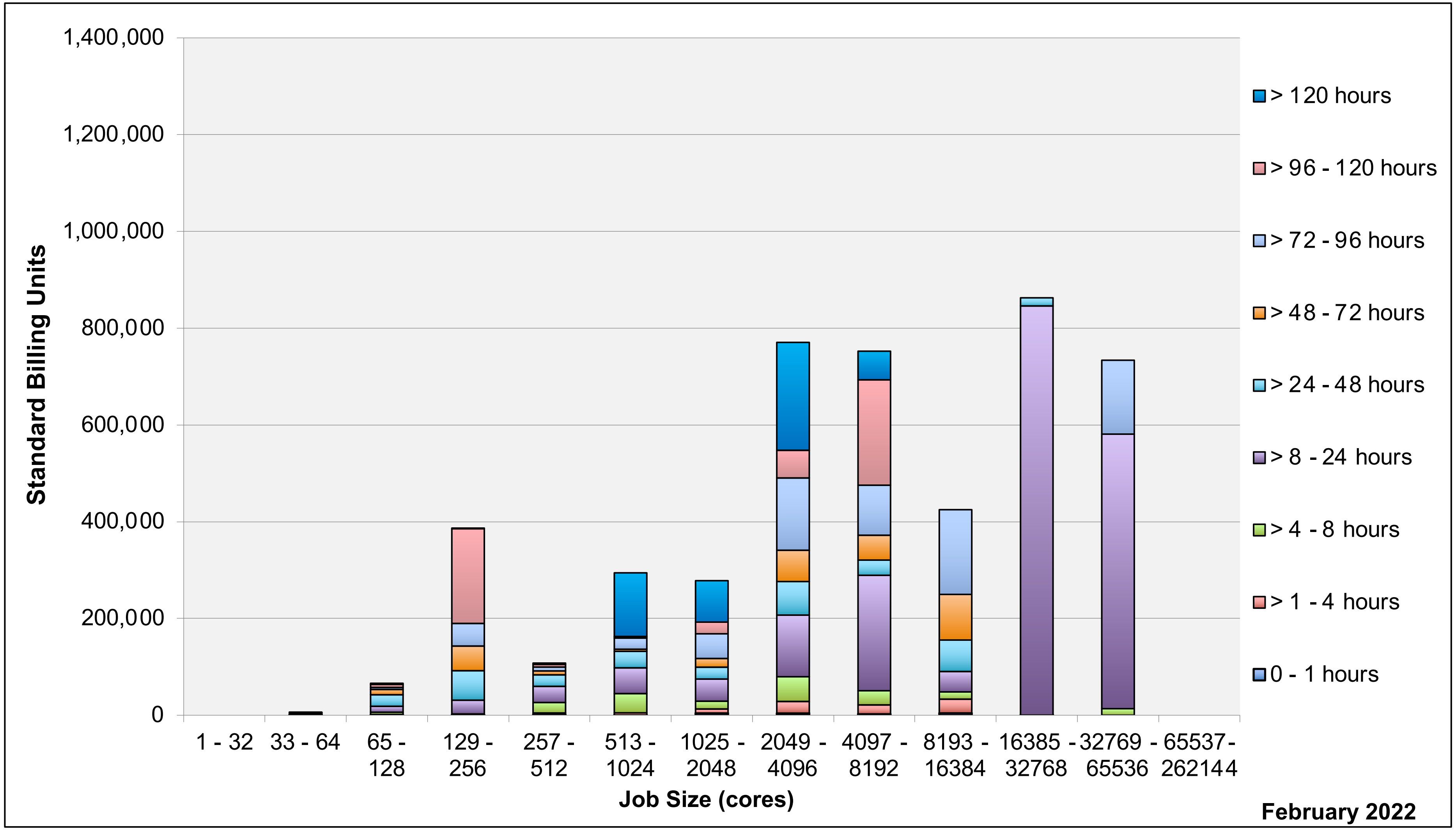
Aitken: Monthly Utilization by Job Length



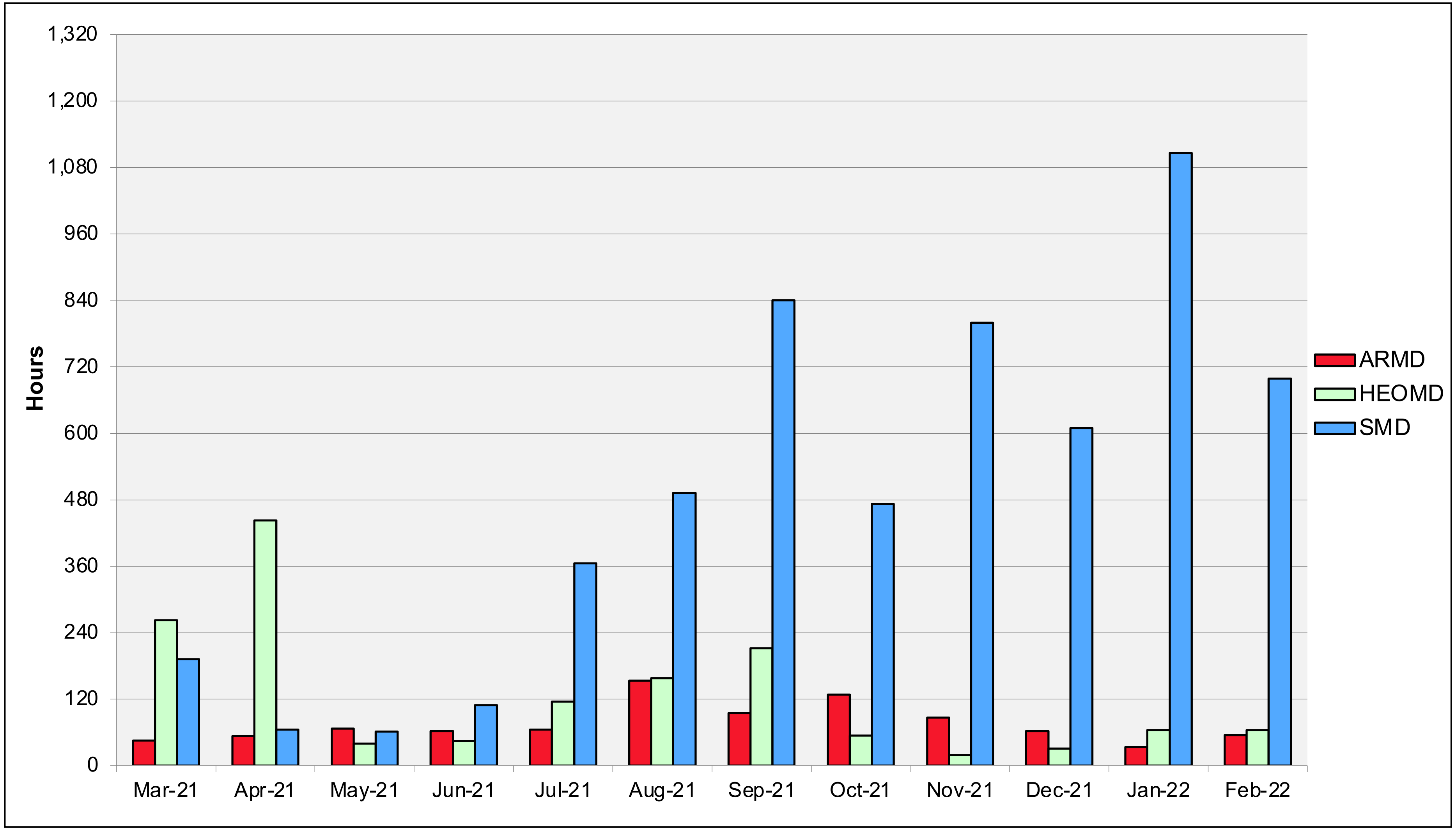
Aitken: Monthly Utilization by Job Size



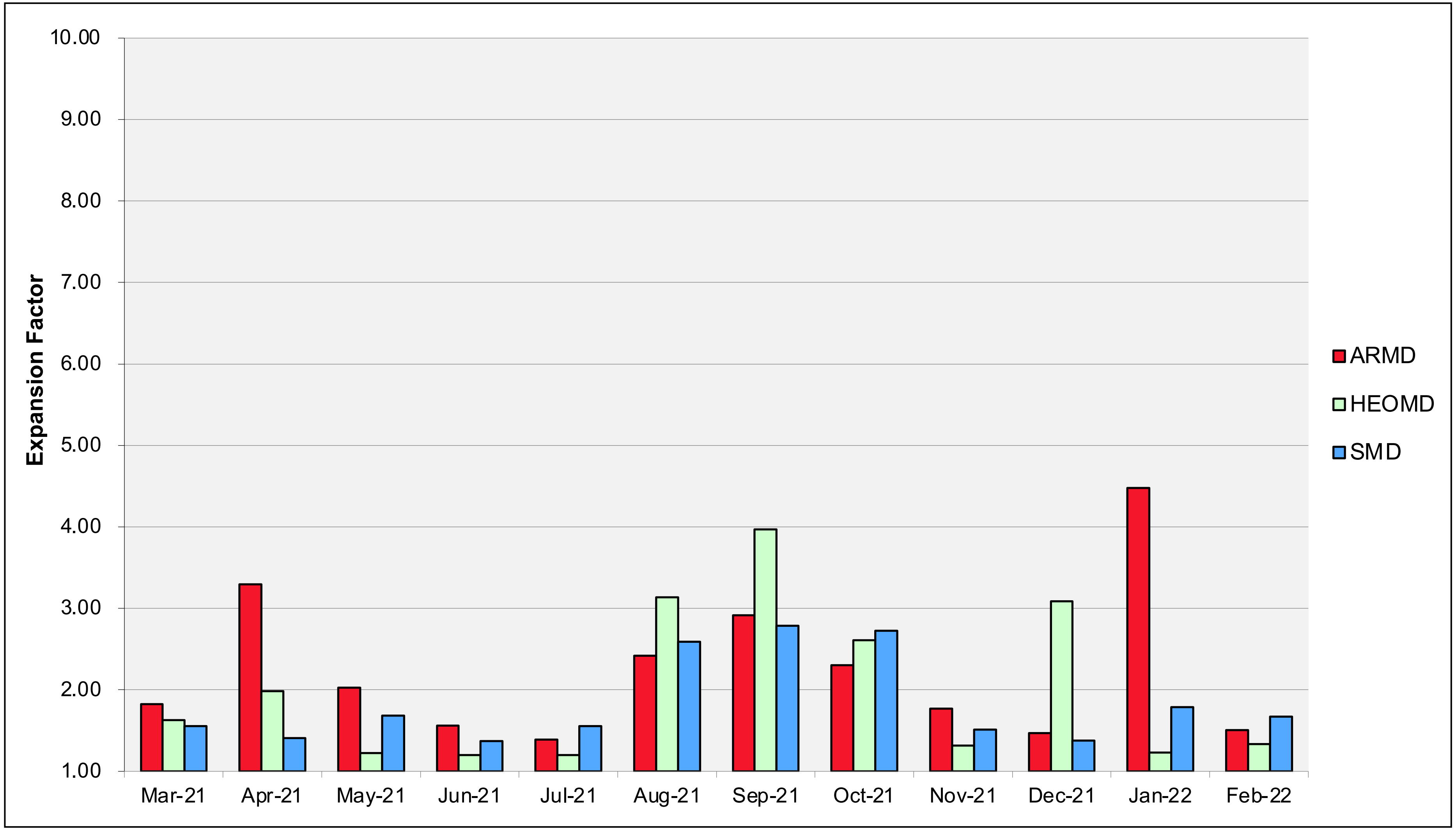
Aitken: Monthly Utilization by Size and Length



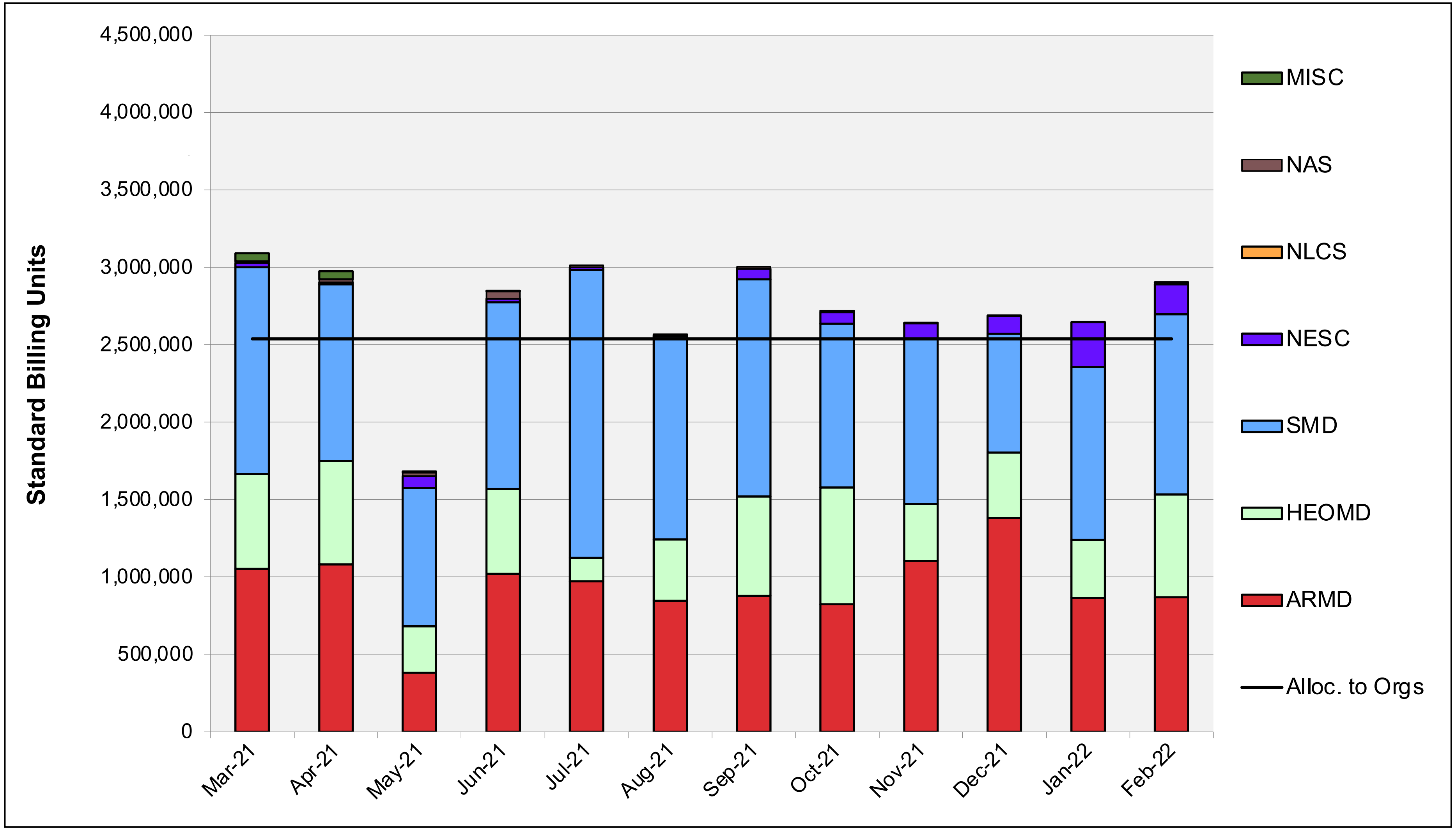
Aitken: Average Time to Clear All Jobs



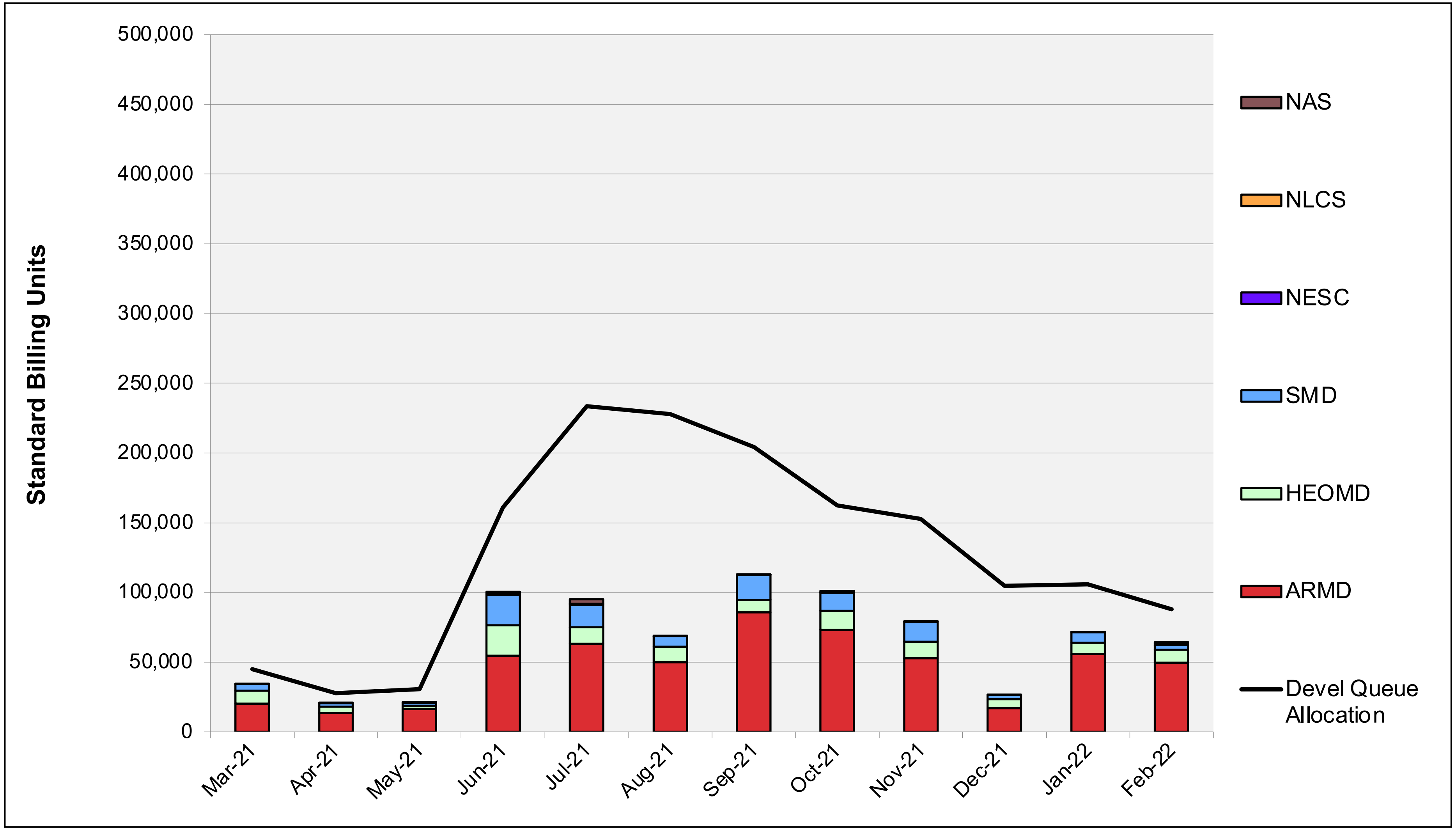
Aitken: Average Expansion Factor



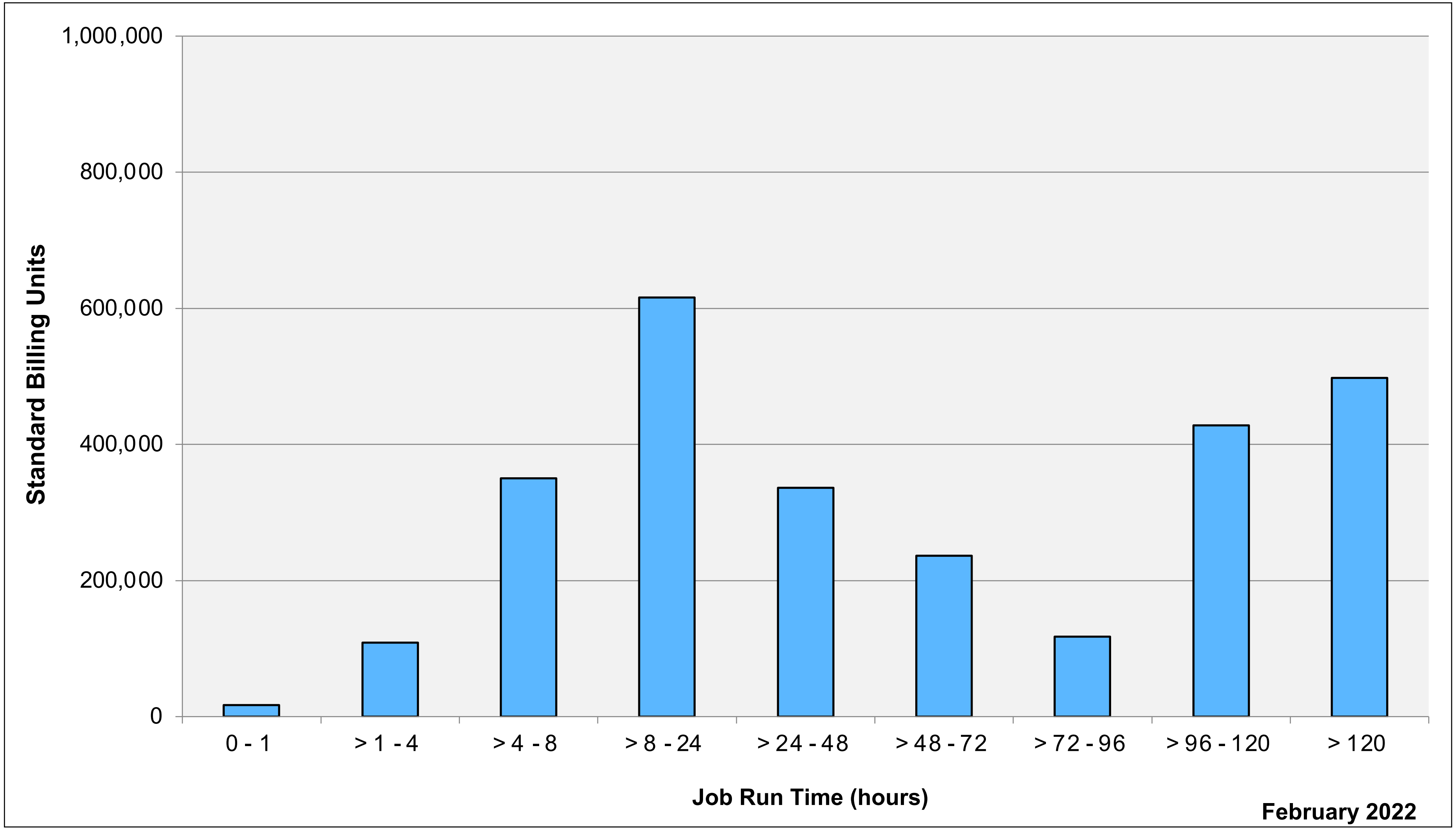
Electra: SBUs Reported, Normalized to 30-Day Month



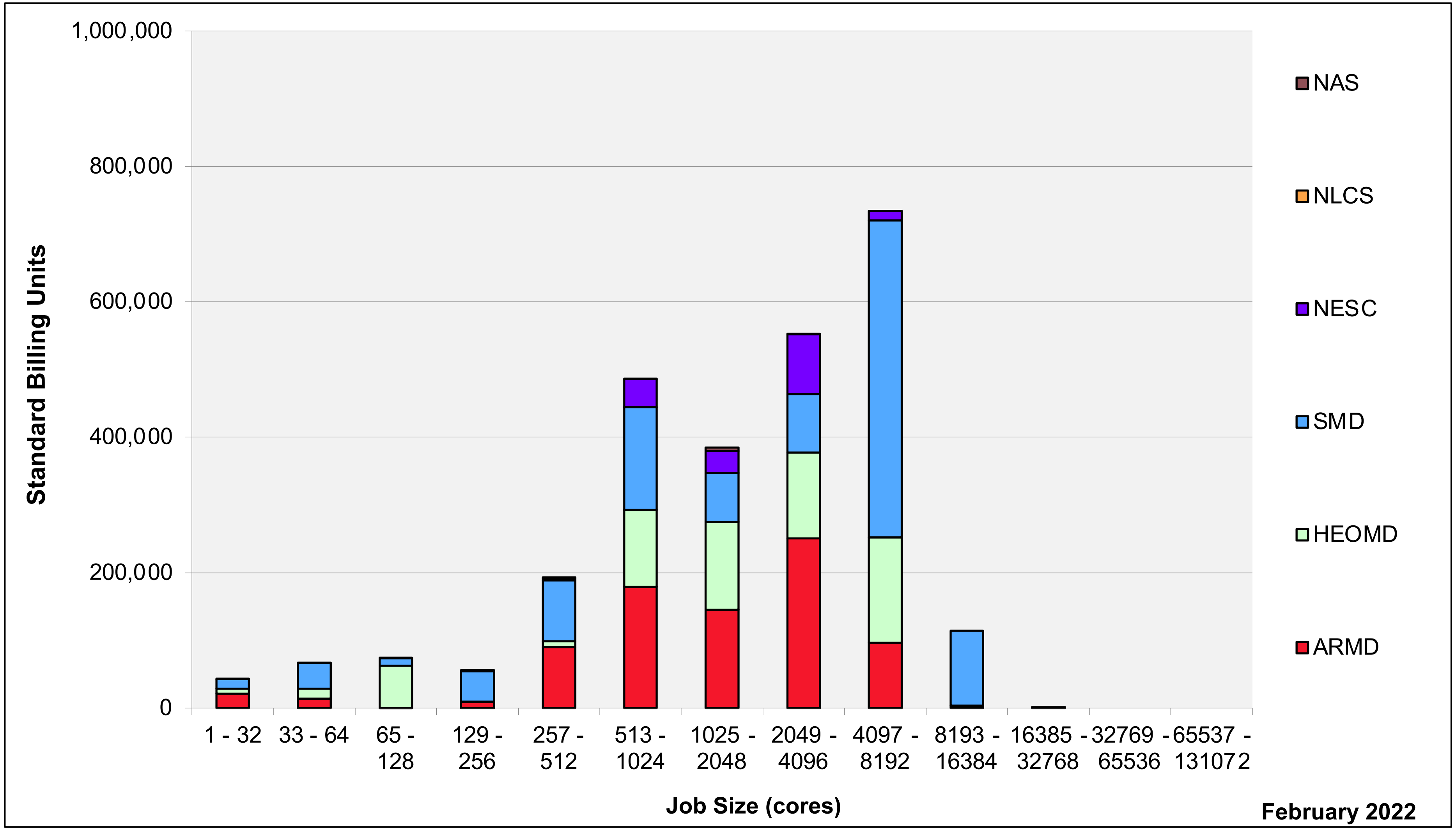
Electra: Devel Queue Utilization



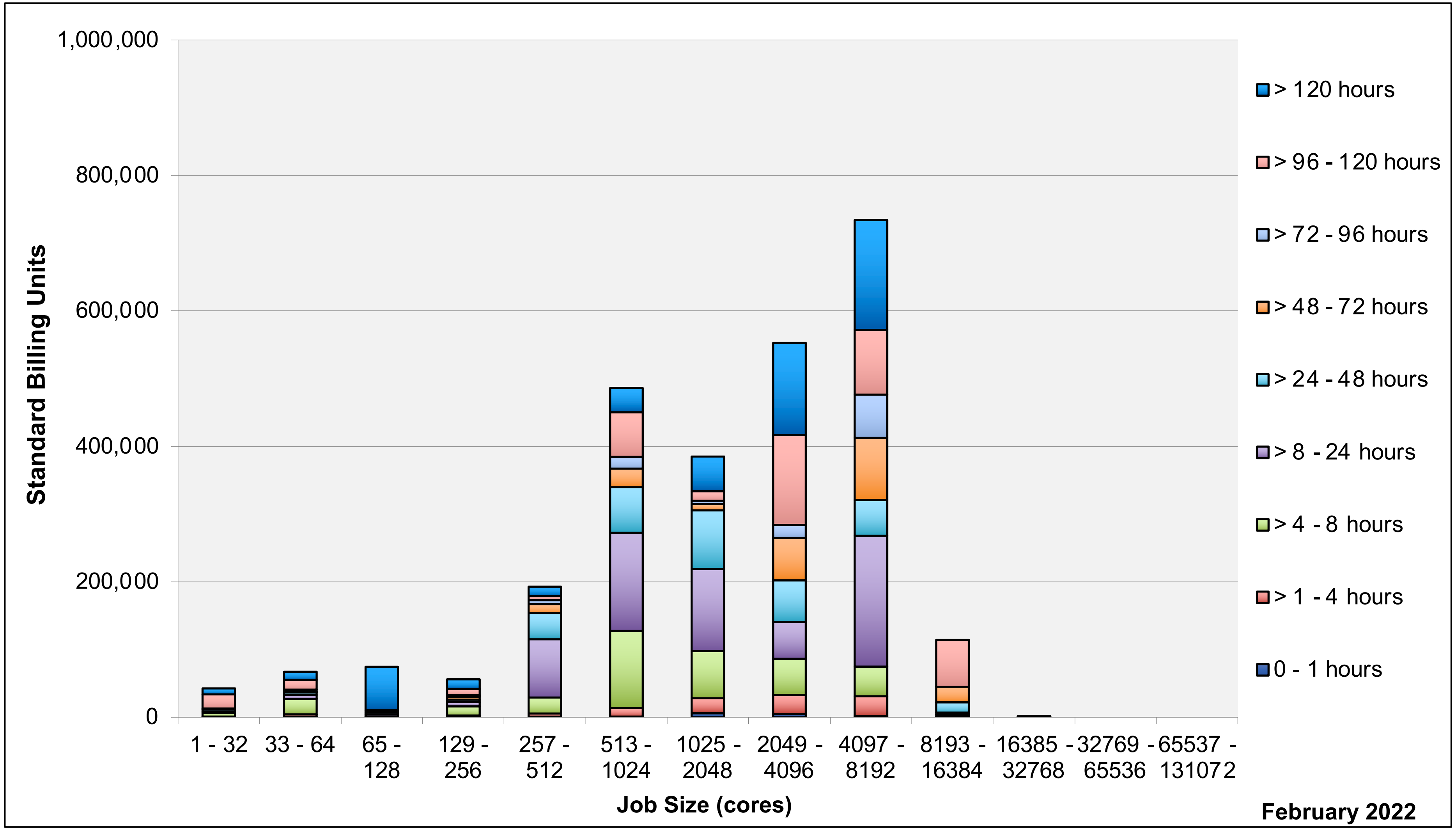
Electra: Monthly Utilization by Job Length



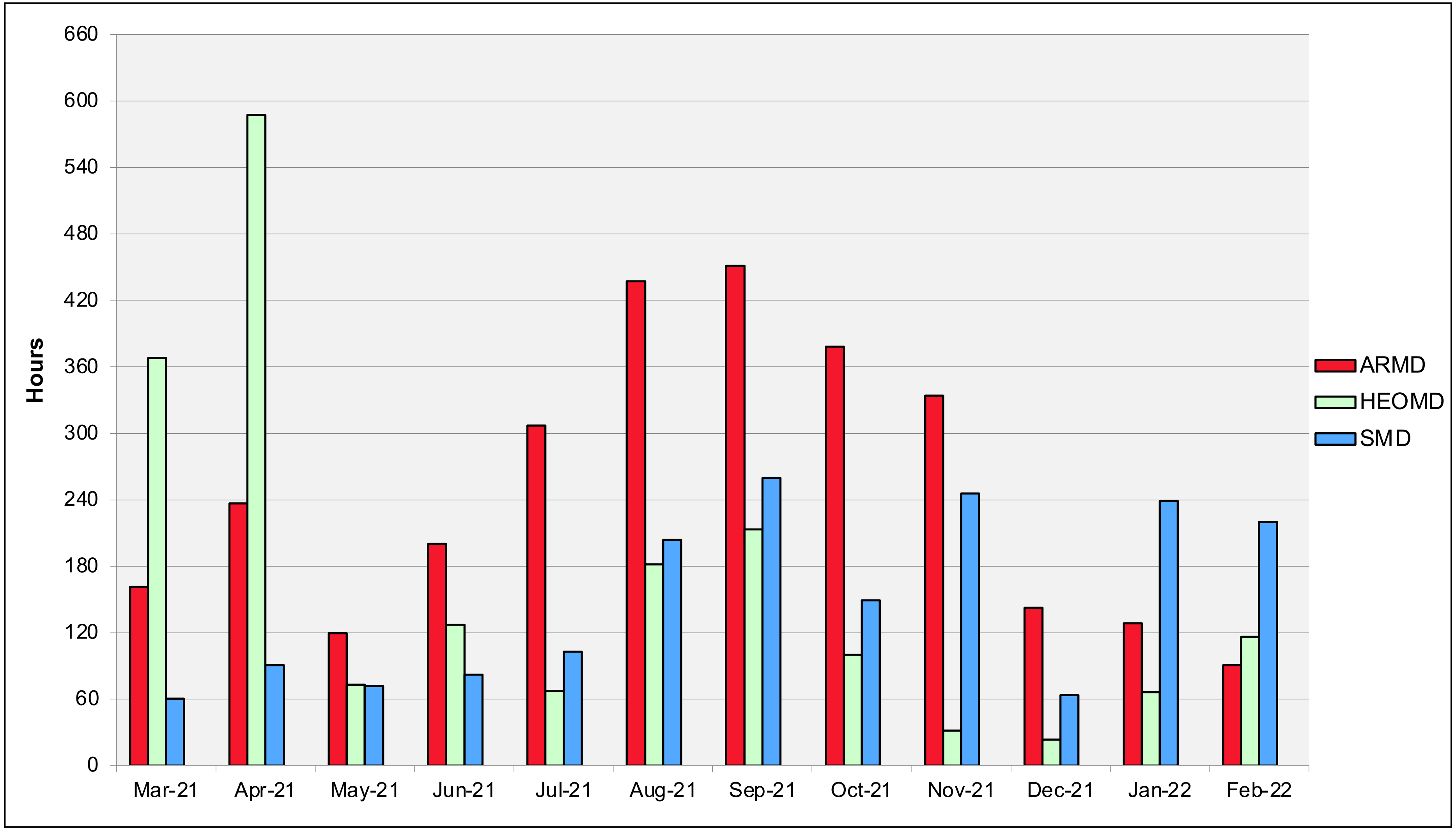
Electra: Monthly Utilization by Job Size



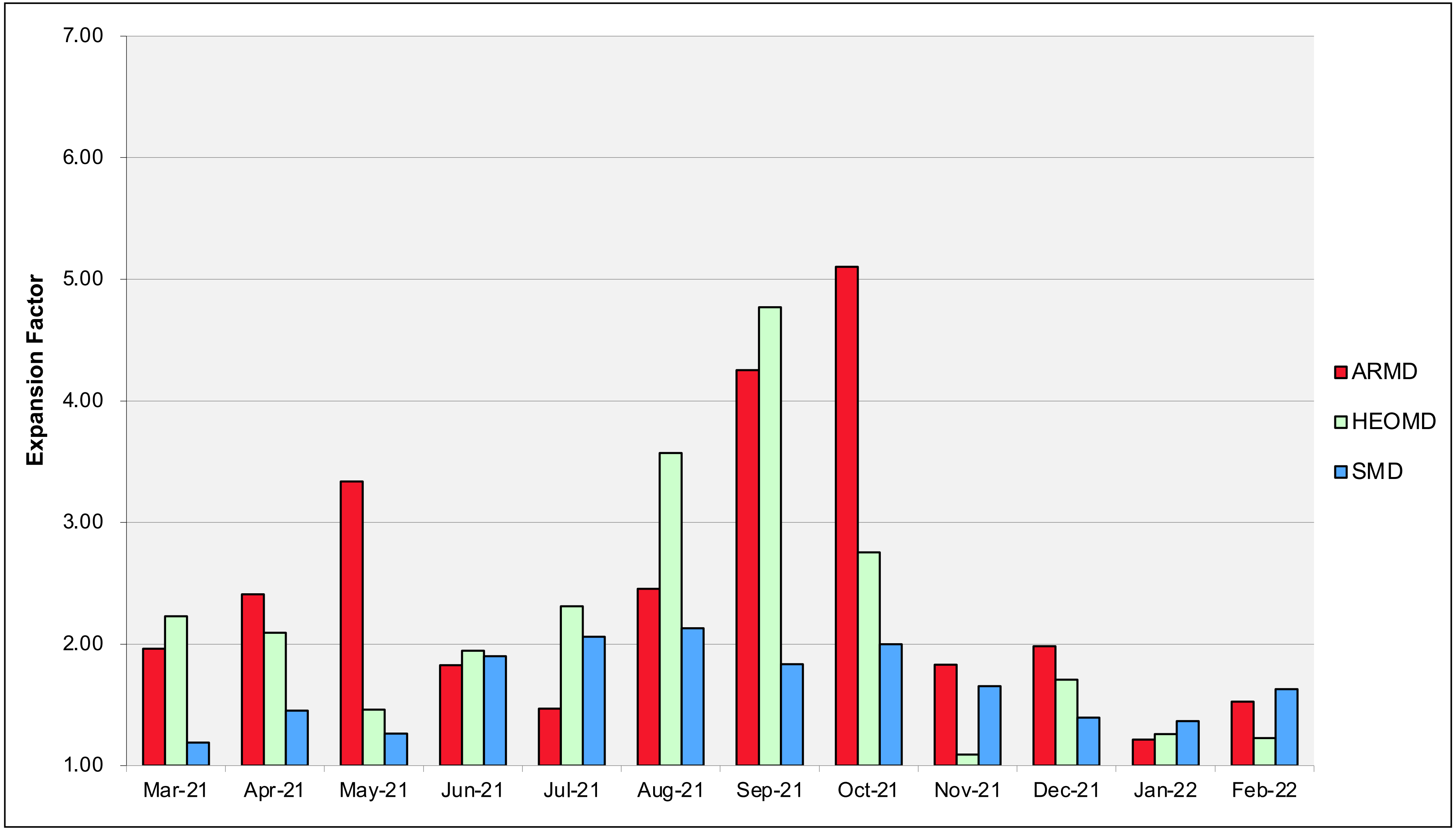
Electra: Monthly Utilization by Size and Length



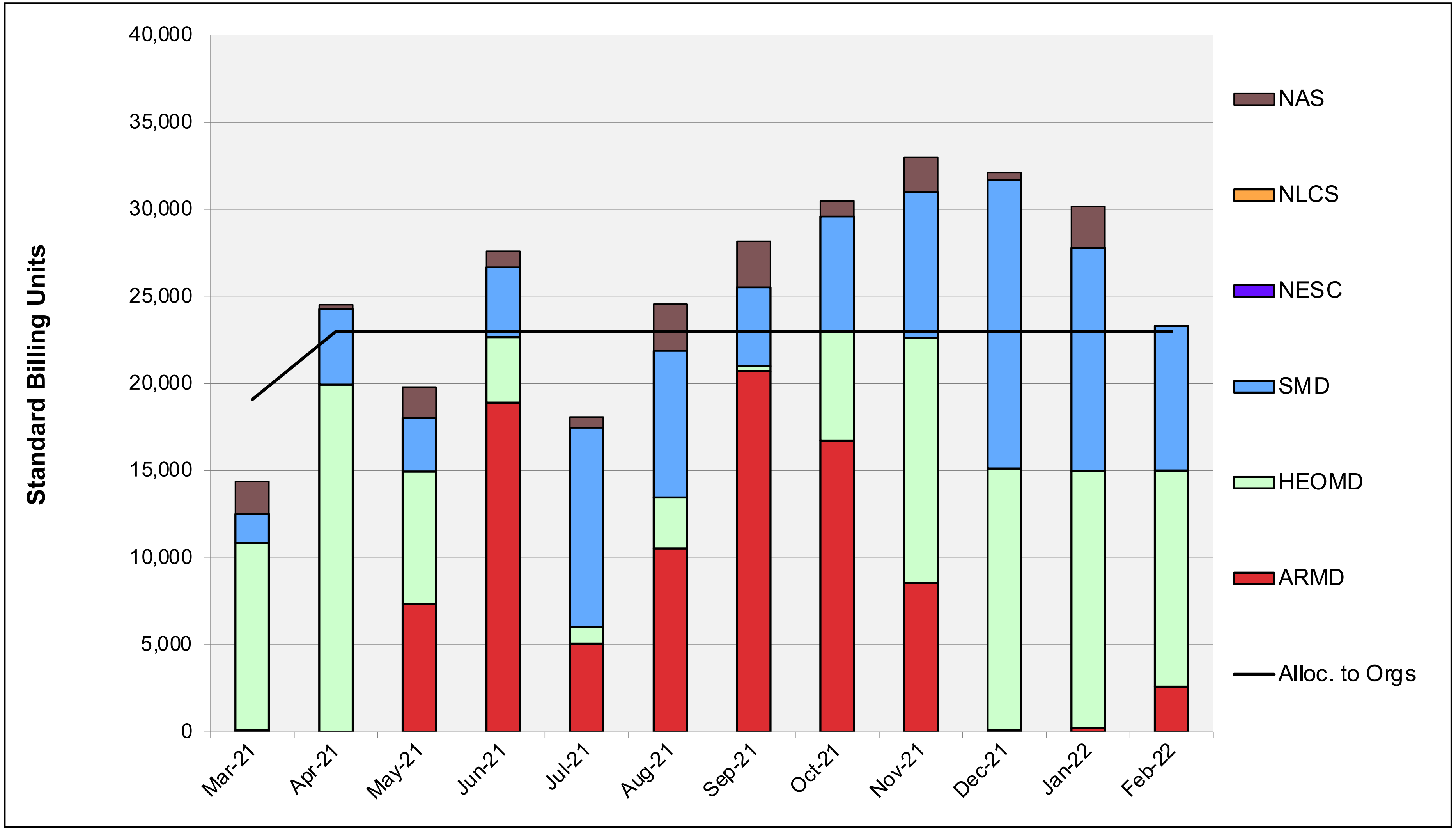
Electra: Average Time to Clear All Jobs



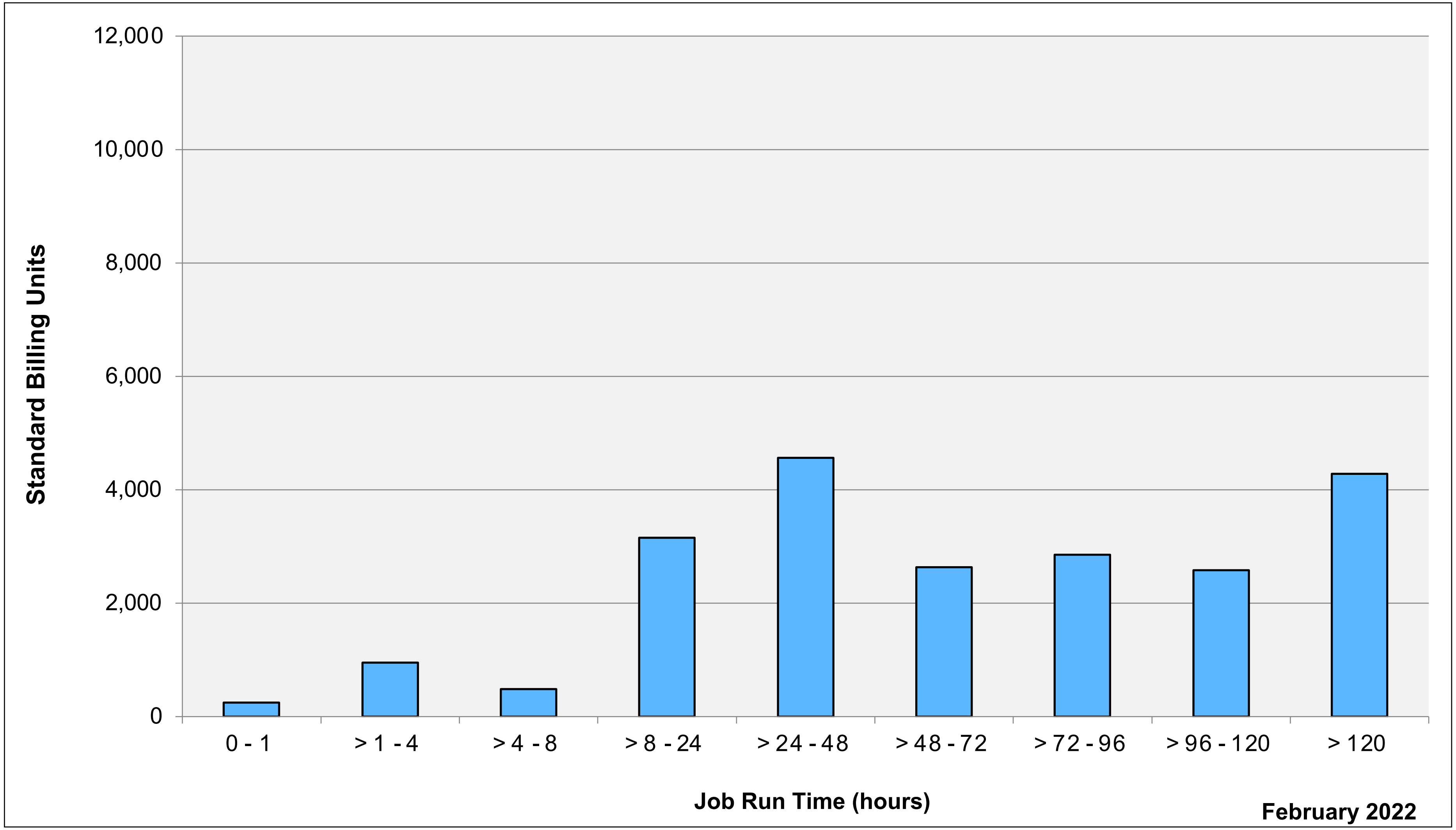
Electra: Average Expansion Factor



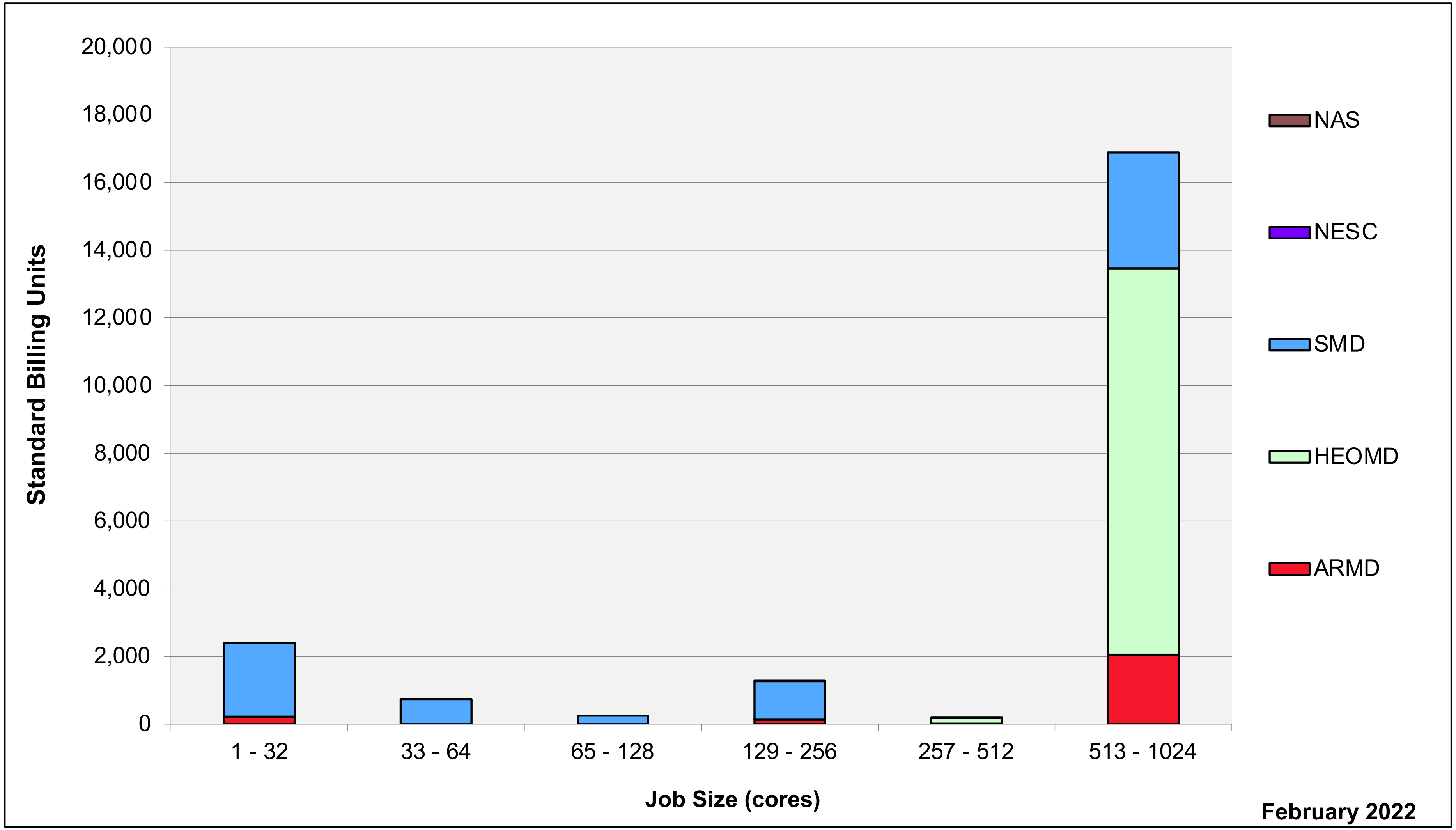
Endeavour: SBUs Reported, Normalized to 30-Day Month



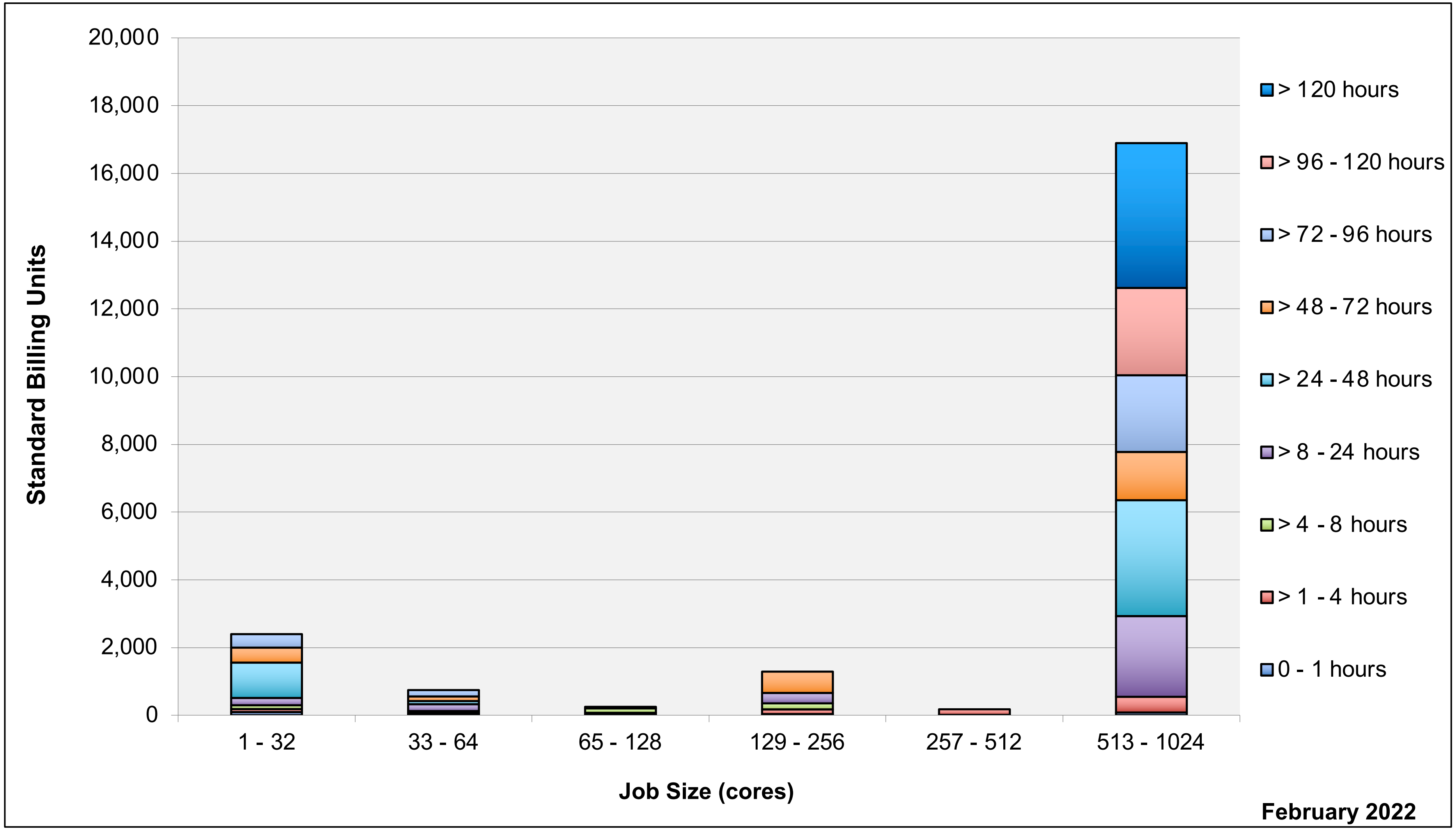
Endeavour: Monthly Utilization by Job Length



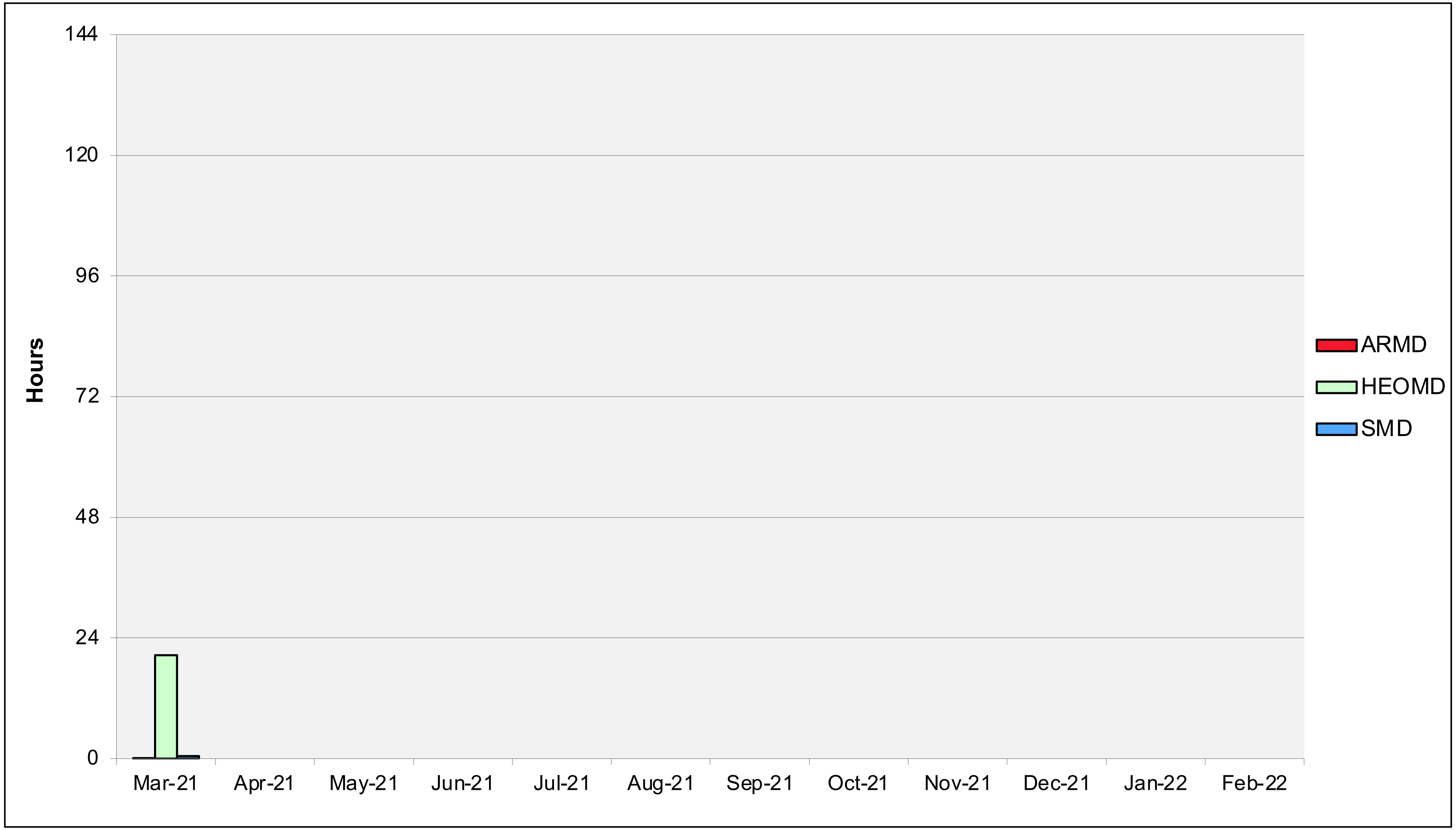
Endeavour: Monthly Utilization by Job Size



Endeavour: Monthly Utilization by Size and Length



Endeavour: Average Time to Clear All Jobs



Endeavour: Average Expansion Factor